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International Collaborations on Fluid Flows in Fractured Crystalline Rocks: FY14 Progress Report

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Executive Summary

Recognizing the benefits of international collaboration in the common goal of safely and efficiently managing the back end of the nuclear fuel cycle, DOE's Office of Nuclear Energy (NE) and its Office of Used Fuel Disposition Research and Development (UFD) have developed a strategic plan to advance cooperation with international partners. Active participation in international R&D is crucial for achieving the UFD long-term goals of conducting "experiments to fill data needs and confirm advanced modeling approaches" (by 2015) and of having a "robust modeling and experimental basis for evaluation of multiple disposal system options" (by 2020). The international collaboration on the evaluation of crystalline disposal media at Sandia National Laboratories (SNL) in FY14 was focused on the following two activities: (1) simulations of flow and transport in Bedrichov Tunnel, Czech Republic as a part of the DECOVALEX program and (2) Korean Atomic Energy Research Institute (KAERI) Underground Research Tunnel (KURT) testing in crystalline rocks. The major accomplishments include:

- DECOVALEX-Bedrichov Tunnel Tests: A lumped parameter model was developed for stable isotope, tritium and CFC-12 transport at the Bedrichov Tunnel site and modeled results were compared to measured data. The lumped parameter model consistently predicts heavier isotopic values observed at the site, indicating preferential recharge of winter precipitation. Code PFLOTRAN was used to simulate multiple environmental tracer concentrations in heterogeneous 2D and 3D domains. Fracture zone permeability was calculated by matching the steady tunnel discharge to the appropriate values given in the task description. The modeling results have demonstrated the potential of using both the lumped parameter model and the PFLOTRAN code for modeling flow and transport in fractured crystalline rocks. The comparison of modeling results among the participating DECOVALEX teams has improved the confidence for the intended use of the modeling tools.

- KAERI Underground Research Tunnel Test: SNL and KAERI have developed a multi-year plan for joint field testing and modeling to support the study of high-level nuclear waste disposal in crystalline geologic media. The work for FY14 is focused on two tasks: (1) streaming potential (SP) testing, and (2) technique development for in-situ borehole characterization. For task 1, KAERI has completed the experimental setup and a first set of preliminary tests. This testing system will be transferred to the underground research laboratory once the new excavation in the KURT is completed. For Task 2, KAERI and SNL have developed a roadmap for the development of site characterization techniques for fractured crystalline rocks, especially the in-situ hydrological and geochemical measurements in boreholes.

- A technical exchange meeting was held under the Joint Fuel Cycle Studies (JFCS) bilateral between the Republic of Korea (ROK) and the US DOE. A list of deliverables for technical data exchange has been identified for next two years.

Future work will include: (1) helping to complete the final technical report for DECOVALEX-2015 Task C; (2) working closely with KAERI on the streaming potential testing in the KURT; (3) planning an actual field test at the KURT site for the development of in-situ measurement techniques in boreholes; and (4) formulating a plan for a joint flow and tracer test at the KURT using the newly excavated tunnel. In addition, we will ensure the delivery of the list of deliverables identified at the JFCS technical exchange meeting.

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1. Objectives

Recognizing the benefits of international collaboration in the common goal of safely and efficiently managing the back end of the nuclear fuel cycle, DOE's Office of Nuclear Energy (NE) and its Office of Used Fuel Disposition Research and Development (UFD) have developed a strategic plan to advance cooperation with international partners (Birkholzer et al., 2013; UFD, 2012). UFD's strategic plan lays out two interdependent areas of international collaboration. The first area is cooperation with the international nuclear community through participation in international organizations, working groups, committees, and expert panels. Such participation typically involves conference and workshop visits, information exchanges, reviews, and training and education. The second area of international collaboration is active R&D participation of U.S. researchers within international projects or programs (UFD, 2012). By active R&D, it is meant that U.S. researchers work closely together with international scientists on specific R&D projects relevant to both sides. With respect to geologic disposal of radioactive waste, such active collaboration provides direct access to information, data, and expertise on various disposal options and geologic environments that have been collected internationally over the past decades. Many international programs have operating underground research laboratories (URLs) in clay/shale, granite, and salt environments, in which relevant field experiments have been and are being conducted. Depending on the type of collaboration, U.S. researchers can participate in planning, conducting, and interpreting experiments in these URLs, and thereby get early access to field studies without having in situ research facilities in the United States.

UFD considers this second area, active international R&D, to be very beneficial in achieving the program's long-term goals of conducting "experiments to fill data needs and confirm advanced modeling approaches" (by 2015) and of having a "robust modeling and experimental basis for evaluation of multiple disposal system options" (by 2020). Advancing opportunities for active international collaboration with respect to geologic disposal has therefore been the primary focus of UFD's international strategy in the recent year (Birkholzer et al., 2013; Birkholzer, 2012).

This report summarizes the work accomplished in FY14 at Sandia National Laboratories (SNL) related to international collaborations on the evaluation of crystalline rocks as disposal media. The FY14 work was focused on the following two activities: (1) simulations of flow and transport in Bedrichov Tunnel, Czech Republic as a part of the DECOVALEX program, and (2) KAERI Underground Research Tunnel testing in crystalline rocks. This work directly supports the following UFD objectives:

- Develop a fundamental understanding of disposal system performance in a range of environments for potential wastes that could arise from future nuclear fuel cycle alternatives through theory, simulation, testing, and experimentation.
- Develop a computational modeling capability for the performance of storage and disposal options for a range of fuel cycle alternatives, evolving from generic models to more robust models of performance assessment.

The work documented here also addresses the following specific topics identified based on the UFD R&D Implementation Plan (Wang, 2013).

- Topic #S5: Evaluation of state of the art of site characterization techniques

- Topic #S7: Identification of the needs for using underground research laboratory
- Topic #P1: Development of discrete fracture network model
- Topic #P2: Parameter estimation and uncertainty quantification of field testing

1.1 References

Birkholzer, J.T. (2012). Status of UFD Campaign International Activities in Disposal Research. Report prepared for U.S. Department of Energy Used Fuel Disposition Campaign, FCRD-UFD-2012-000295.

Birkholzer, J., Asahina, D., Chen, F., Gardner, P., Houseworth, J., Jove-Colon, C., Kersting, A., Nair, P., Nutt, M., Li, L., Liu, H.H., Painter, S., Reimus, P., Rutqvist, J., Steefel, C., Tynan, M., Wang, Y., Zavarin, M. (2013). An overview of US disposal research activities linked to international URLs. Proceedings of the 2013 International High-Level Radioactive Waste Management Conference (IHLRWM), April 28 – May 2, 2013, Albuquerque, New Mexico.

UFD (2012). Office of Used Fuel Disposition International Program — Strategic Plan (2013) April 2012, U.S. Department of Energy.

Wang, Y. (2013) Research &Devlopement (R&D) Plan for Used Fuel Disposition Campaign (UFDC) Natural System Evaluation and Tool Development (Rev 1).

2. Simulation of Flow and Transport in Bedrichov Tunnel, Czech Republic

Fluid flow and transport in fractures have been identified to be an important issue for nuclear waste disposal in crystalline rocks (Wang, 2013). Environmental tracers are non-applied chemical species present in precipitation with known concentration histories and known decay and production rates in the subsurface. These tracers provide information on the transport characteristics of groundwater systems over a wide range of time scales. The primary goal of this study is to use environmental tracer data from the Bedrichov tunnel experiment to help characterize fracture transport characteristics. Cutting-edge transport theory and computational power are being used to incorporate environmental tracer information in estimating fracture network capabilities. The primary activities accomplish during FY-2014 include attending the Development of Coupled Models and their Validation against Experiments (DECOVALEX)-2015 meeting in Avignon, France, using computer code PFLOTRAN to simulate tracer transport at Bedrichov site, and help develop the first draft of a technical report DECOALEX-2015 Task C2 – Bedrichov Tunnel Test Case.

The Bedrichov tunnel is located in Jizera Mountains, north of the Czech Republic, part of the Bohemian Massif, Krkonoše-Jizera Composite Massif (Figure 2-1). The tunnel is about 1 km in length with a max depth of 200 m and cuts through fractured granite. The tunnel was excavated during 1980-1981, the first 890m from the southwest with a tunnel boring machine and the remaining part by a drill-and-blast method. The last part of ~150 m on the reservoir bottom was constructed from the surface. The research related to nuclear waste repository development at the Bedrichov site started in 2003, with support of RAWRA, led by J. Klomínský from Czech Geological Survey, with the participation of several other institutes. The site is important as one of the few underground research facilities in hard host rocks in the Czech Republic.

Task C2 of the DECOVALEX-2015 is centered around a dataset of environmental tracers and discharge in Bedrichov Tunnel. The dataset were mostly obtained by Technical University of Liberec (TUL), but some part of it was obtained by other participating organizations. The dataset includes stable isotopes of water, tritium, tritiogenic ^{3}He and other noble gases, and dissolved chlorofluorcarbons (CFC's) measured in fracture discharge. It leverages an existing data collection point for stable isotopes and tritium measured in precipitation near the study site. The goal of Task C2 is to model groundwater flow and transport of environmental tracers in the fractured system surrounding the Bedrichov Tunnel, and utilize this data to constraint fracture network parameters.

This section summarizes the accomplishments up to date jointly by all participating organizations for the DECOVALEX Task C2. The text that follows is mainly taken from the draft of technical report recently assembled for the task.

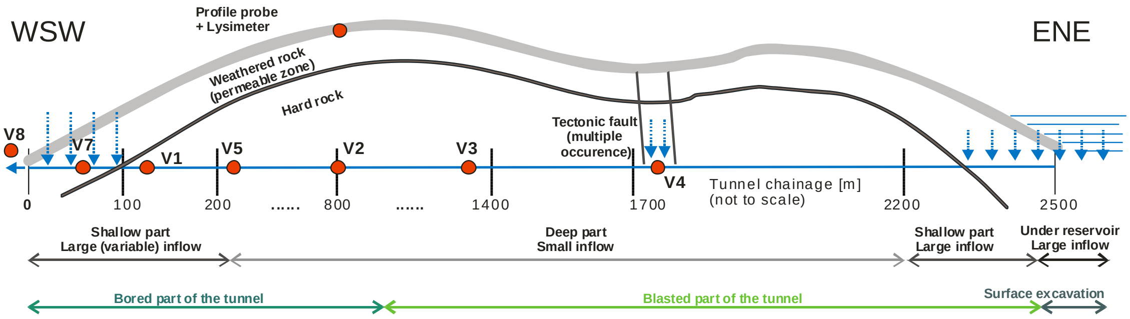


Figure 2-1: Tunnel profile – technical and hydrogeological conditions

2.1 Problem definition

A model has been developed to represent a part of the tunnel at a particular depth, without an explicit consideration of exact terrain shape, as illustrated in Figure 2-2. Use of symmetric quarter for numerical solution is recommended. An effect of mixing water from slow flow through the massif and fast flow through a fracture/fault is included. Also, the division of shallow more permeable and deep less permeable parts is necessary and described below. The dimension of the modeling domain is chosen as follows: 600 m width perpendicular to the tunnel (300 m for symmetric model), 400 m depth and 200 m width along the tunnel (100 m for symmetric model – on each side of the fracture. The particular solution can include any of the equivalent continuum, discrete fracture network, and hybrid models (with different representations of the more and less conductive domains), but the overall goal is aimed at the combination of a 3D domain of rock continuum and a 2D domain of fault/fracture.

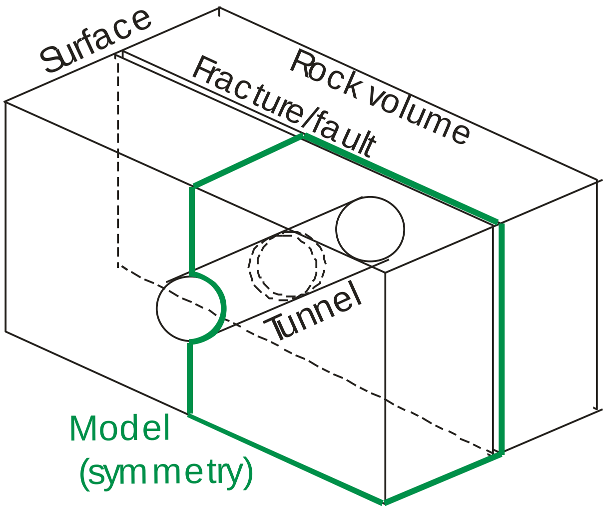


Figure 2-2: Conceptual model for particular place in the tunnel distinguishing the inflow from a fracture/fault and rock continuum (matrix or network of smaller fractures).

Four particular configurations are considered to represent typical tunnel segments around inflow measurement positions (Figure 2-3):

- Model 1: interval 0-100 m (shallow weathered layer), inflow measurement position at 70 m (V7), aggregating all inflow in the real segment
- Model 2: interval 100-250 m (hard rock just below the shallow weathered zone), inflow measurement positions at 125 m (V1 – drops from a single fracture), 142 m (larger inflow from a fracture set), 225 m (single fracture with continuous flow)
- Model 3: position at 798 m (deep in compact rock, weak inflow) – measurement at V2 (drops)
- Model 4: position at 1728 m (deep, fault zone 5-20 m width) – measured at V4

Three basic components of the model are defined: a 3D shallow zone with the hydraulic conductivity K_1, a 3D deep zone with the hydraulic conductivity K_2 and a vertical fracture or fault with the transmissivity T_f (possibly evaluated from a given thickness and hydraulic conductivity). In each scheme, the left part is a vertical section along the tunnel (grey strip) and the right part is a vertical section perpendicular to the tunnel (grey circle).

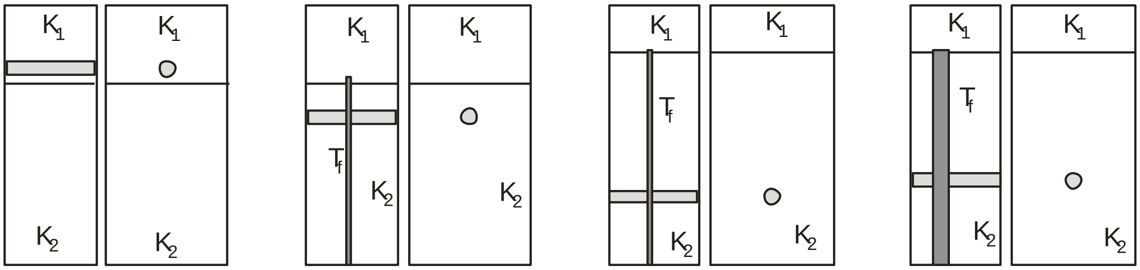


Figure 2-3: Particular model configuration (1-4) representing selected real positions in the tunnel (for the numerical discretization, it is convenient to consider the fracture/fault domain up to the surface).

Three issues considered in constraining the boundary conditions for modelling:

- The water level is not measured and its calculation from infiltration/recharge is only possible for a realistic topography in a larger scale. The prescribed water level in the upper domain on the outer side from the tunnel provides a necessary reference while directly above the tunnel the water level can vary with seasonal conditions and influence the tunnel inflow. On the other hand, the flow below is vertical as deduced from the model scale (see Figure 2-4).
- It is necessary to prescribe the real value of infiltration/recharge to have correct balance of natural tracers or to incorporate the role of shallow zone in draining the excessive or supplying the missing water expected for the tunnel inflow.
- The intended vertical flow (existing without the tunnel influence) in the deeper part cannot be realistically controlled by infiltration (which is redistributed in the shallow zone), and it must be evaluated from prescribed estimation of pressure gradient – the

pressure or piezometric head value on the bottom boundary is derived from the scale proportions – the difference of 200 m altitude (and piezometric head) between the highest and the lowest point along the 1000 m distance corresponds to 80 m difference between the model top and bottom (-80 m head value prescribed).

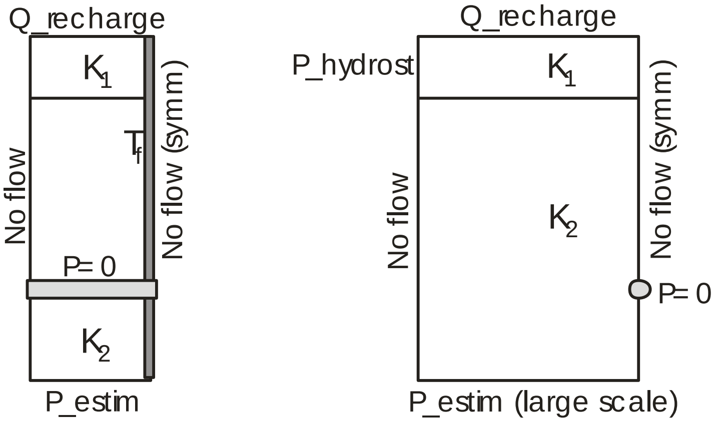


Figure 2-4: Boundary conditions for the 3D tunnel inflow model – the left is a view perpendicular to the tunnel and the right is along the tunnel

2.2 Contribution of TUL

2.2.1 Multidimensional approach

The conceptual model used combines the ideas of equivalent continuum model, discrete fracture network, and double-porosity model. We consider a system of 3D continuum, 2D discrete fracture network and a network of 1D fracture intersection. Each part is further composed of a mobile and immobile part (double continuum). The interpretation of each of the six zones is the following (see Figure 2-5):

- 3D mobile zone: rock pores, equivalent continuum representation of small fractures;
- 3D immobile zone: dead-end pores in rock, immobile zone of double-porosity representation of small fractures;
- 2D mobile zone: discrete fracture network of large fractures, or representation of planar structures of similar behavior (e.g. a fracture zone as a single plane in a larger scale). In case of the representation by double porosity model, only the mobile zone is considered.
- 2D immobile zone: dead-end pores if the fracture is filled with minerals, immobile zone of the representation of a general planar structure with the single-plane double porosity model (above)
- 1D mobile zone: intersections of discrete fractures;
- 1D immobile zone: like 2D immobile zone in the 2D model geometry with 1D fractures (not a typical case in 3D models)

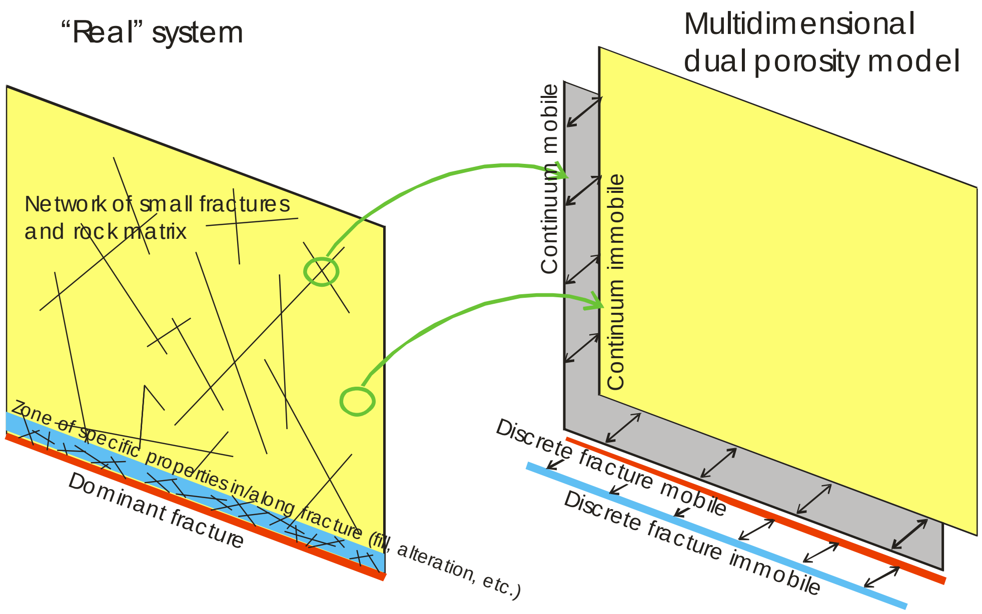


Figure 2-5: Scheme of interpretation of each dimension of multi-dimensional model with immobile zones

We assume that the fluid flow in each subdomain (dimension) is governed by the Darcy law, i.e., potential flow in each 1D, 2D, and 3D domain. This is consistent with the standard Darcy law for 3D continuum and the Hagen-Poiseuille law for flow in open fracture, with appropriate real or equivalent hydraulic conductivity. The interaction between domains is consistently represented by corresponding linear flux-pressure relation (transmissivity coefficient σ). The transport problem is governed by the advection-diffusion (hydrodynamic dispersion) equation coupled with linear law of non-equilibrium exchange between mobile and immobile zone. The transport between the 1D, 2D and 3D domains is included in the advection term. Nuclear and chemical reactions are represented as additional source terms in both zones.

We denote the problem domain $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$, $\Omega_i \subset R_3$, $i = 1,2,3$, where Ω_3 is polyhedron (3D continuum), Ω_2 is a system of planar polygons (discrete fracture network) and Ω_1 is a systems of lines (intersections of fractures = "pipes"). We define the mixed Dirichlet (a prescribed piezometric head) and Neumann (a prescribed flux) boundaries $\partial\Omega_i = \Gamma_{i,D} \cup \Gamma_{i,N}$, $\Gamma_{i,D} \neq \varnothing$, $\Gamma_{i,D} \cap \Gamma_{i,N} = \varnothing$. The governing equations of flow (see also Maryška et al. (2008) for more details) are

$$\vec{u}_i = -K_i \nabla p_i \quad in\ \Omega_i \tag{2.1}$$

$$\kappa_i \frac{\partial p_i}{\partial t} - \nabla \cdot \vec{u}_i = q_i^+ + q_i^- + \sum_{j=1,\, j\neq i}^{3} \frac{\tilde{q}_{ij}}{\mu_i} \quad in\Omega_i \tag{2.2}$$

$$p_i = p_{i,D} \quad on\Gamma_{i,D} \tag{2.3}$$

$$\vec{u}_i \cdot \vec{\nu}_i = u_{i,N} \quad on\Gamma_{i,N} \tag{2.4}$$

$$\tilde{q}_{ij} = \sigma_{ij}(p_i - p_j) \qquad i \neq j \tag{2.5}$$

$$i = 1, 2, 3$$

where the unknowns are $u_i(\vec{x},t)$ - the velocity and $p_i(\vec{x},t)$ - the piezometric head; the parameters K_i is the hydraulic conductivity, κ_i the storativity, q_i sources/sinks, σ_{ij} transmissivity between domains. The auxiliary variable $\tilde{q}_{ij}$ denotes the flux between domains of different dimensionality (positive from j to i). The boundary values are $p_{i,D}$ - the pressure head and $u_{i,N}$ - the flux. The additional dimension μ_i ensures the compatible physical dimension of all variables: μ_1 is cross-sectional area of 1D domain, μ_2 is thickness of 2D domain, and $\mu_3 = 1$. On the other hand, the thickness is not considered when defining the positions and intersections of fractures.

The governing equations of the solute transport are

$$n_i^{(m)} \frac{\partial c_i^{(m)}}{\partial t} = -\nabla \cdot (c_i^{(m)} \vec{u}_i) + \nabla \cdot (\mathbf{D}_h^{(i)} \nabla c_i^{(m)}) + \tag{2.6}$$

$$q^+ c^{(m)*} + q^- c^{(m)} + \sum_{j=1,\, j\neq i}^{3} \frac{\tilde{q}_{ij}^{(c)}}{\mu_i} + r_i^{(m)} - \alpha_i (c_i^{(m)} - c_i^{(im)})$$

$$n_i^{(im)} \frac{\partial c_i^{(im)}}{\partial t} = r_i^{(im)} + \alpha_i (c_i^{(m)} - c_i^{(im)})$$

$$[\mathbf{D}_h]_{kl} = \delta_{kl} D_m + \alpha_T . |\mathbf{u}| . \delta_{kl} + (\alpha_L - \alpha_T) \frac{u_k u_l}{|\mathbf{u}|}, \tag{2.7}$$

where the unknowns are $c^{(m)}$ - mobile concentration and $c^{(im)}$ - immobile concentration, the parameter c^* is the injected concentration, $\tilde{q}_{ij}^{(c)}$ the auxiliary solute source/sink due to the interaction between domains,

$$\tilde{q}_{ij}^{(c)} = \begin{cases} \tilde{q}_{ij} c_j^{(m)} & for \tilde{q}_{ij} > 0 \\ \tilde{q}_{ij} c_i^{(m)} & for \tilde{q}_{ij} < 0 \end{cases} \tag{2.8}$$

D_h is the tensor of hydrodynamic dispersion, α rate of mobile-immobile exchange, α_L, α_T longitudinal and transversal dispersivity, $r_i^{(m)}$, $r_i^{(im)}$ chemical reaction production terms, i, j dimension of the domain – subscript at the corresponding unknown.

2.2.2 Flow123D software

The mixed-hybrid finite element method was used, with the lowest-order Raviart-Thomas base functions on tetrahedras (3D subdomain), triangles (2D subdomains), and line segments (1D) (i.e. piecewise linear functions) for the velocity unknown, while the pressures are approximated by piecewise constant function. The discrete unknowns are the fluxes between the elements, the pressures at the element centres, and that pressures at the element side centres. In this way, an approximation of both the unknowns $p_i(x, t)$ and $u_i(x, t)$ is obtained at the same time, with a better regularity for the velocity, including the discrete mass balance property.

The particular adjustment for the multidimensional domain is presented in (Maryška et al., 2008). The side pressures of the 3D elements are coupled with the element pressures of the coinciding 2D elements. In the contact of more 2D elements in the space, the additional boundary balance condition comprises all such discrete fluxes associated with the element sides. The scheme for the discrete unknown positions and connections is illustrated in Figure 2-6, for the 1D-2D analogy.

The discretization leads to an indefinite system of linear algebraic equation which is solved by the Schur complement method – transforming to the system with symmetric positive definite matrix.

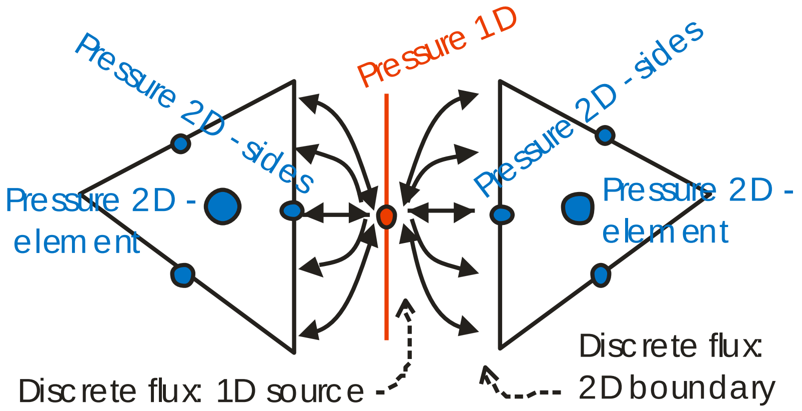


Figure 2-6: Scheme of the discrete unknowns in the multidimensional mixed-hybrid finite elements

The method is implemented in the open-source code FLOW123D developed at the Technical University of Liberec (TUL, 2012). Basic algebraic operations are based on the PETSc library, including the option of parallelization. The code works in the command line regime and uses the

GSMH and ParaView programs for pre- and post-processing. A new option of SALOME software for the geometry preprocessing is also introduced. The code has been formerly verified for the solution of several simple problems against analytical solutions listed in the developers' documentation.

2.2.3 Lumped parameter model and software

For steady flow through a groundwater system, the output concentration *C(t)*, can be related to the input concentration $C_{in}(t')$ of any tracer by the well-known convolution integral (Equ. 2.9), which is implemented in the software FLOWPC (Maloszewski and Zuber, 1996). The lumped-parameter approach is usually limited to one- or two-parameter models. The type of the model and its parameters define the exit-age distribution function (the weighting function) which gives the spectrum of the transit times (Maloszewski and Zuber, 1996). The dispersion function was chosen for this study (Equ. 2.9):

$$C(t) = \int_{-\infty}^{0} C_{in}(t')g(t-t')e^{\left[-\lambda(t-t')\right]}dt \tag{2.9}$$

where *t'* is time of entry , and *t - t'* is the transit time. The type of model is defined by the *g(t')* function:

$$g(t') = \left(\frac{4\prod t^3}{Pe\,t_t}\right)^{-1/2} \cdot e^{\left[-\left(\frac{1-t'}{t_t}\right)^2 t_t \frac{Pe}{t'}\right]}, \tag{2.10}$$

where Pe is the so-called Peclet number. The reciprocal of Pe is equal to the dispersion parameter, $Pe^{-1}=D/vx$, where *D* is the dispersion coefficient.

The lumped parameter approach uses *mean transit time* for modeling of a moving tracer. The artificial pulse in advection model was considered equivalent to the transit time of the lumped parameter approach. The general definition of the transit time is (Maloszewski and Zuber, 1996):

$$t_t = \int_0^{\infty} tC_I(t)dt \Big/ \int_0^{\infty} C_I(t)dt \tag{2.11}$$

where $C_I(t)$ is the tracer concentration observed at the measuring point and the result of an instantaneous injection at the injection point at $t = 0$.

2.2.4 Estimation of water age from stable isotopes

Lumped parameter calibration of water residence time of stable isotopes $d^{18}O$ and d^2H was extended until June 2013. Generally the observed seepage sites near the entrance (drainage 0-142) could be successfully calibrated and the water residence time was from 34 to 44 months. These seepage sites are probably affected by weathered rock. Other seepage sites in the hard rock could not be calibrated (model efficiency was under zero). The time series of measurements is probably shorter compared to the residence time of stable isotopes in outflow water. The seepage sites near the dam with residence time from 53 to 63 month could be influenced by the reservoir with a complicated mixing regime (Table 2-1).

Figure 2-7 A depicts the calibration of d18O of the groundwater seepage site V7 (76 m position) until 6/15/2013. The previous residence time was shorter in the last calibration and the model efficiency was higher. Comparison of four previous calibrations of V7 is shown in Table 2-2 and in Figure 2-7B. It shows how the larger set of measured data changes the optimal fitting model, i.e. the uncertainty related to the calibration.

Table 2-1: Results of estimation of residence time (bold numbers) of the seepage sites calibrated by lumped parameter model (FLOWPC) from $\delta^{18}O$ data. Only the first three columns are relevant fits.

Position	V7	V1	V6	V5	V2	V3	W1565	V41	V42	W2210	W2313	W2470
Outflow[ml/s]	0-200	0.02	10	3	0.03	0.02	12	14	8	22	20	33
Depth [m]	-23	-36	-41	-61	-140	-118	-107	-90	-90	-71	-59	-35
Chainage [m]	76	125	142	226	798	1375	1565	1728	1727	2210	2313	2470
Dispersion par.	0.41	0.25	0.38	0.4	0.39	0.34	0.32	0.34	0.39	0.25	0.37	0.78
R.time [month]	**34**	**43.7**	**37.3**	**31.8**	**37.9**	**37.5**	**53.3**	**37.3**	**50.1**	**58.5**	**52.4**	**62.3**
Model effic.[%]	63.1	63.7	63.3	15.5	0	0	0	0	0	0	0	0
Sigma	0.022	0.019	0.02	0.034	0.035	0.036	0.23	0.043	0.24	0.03	0.027	0.045

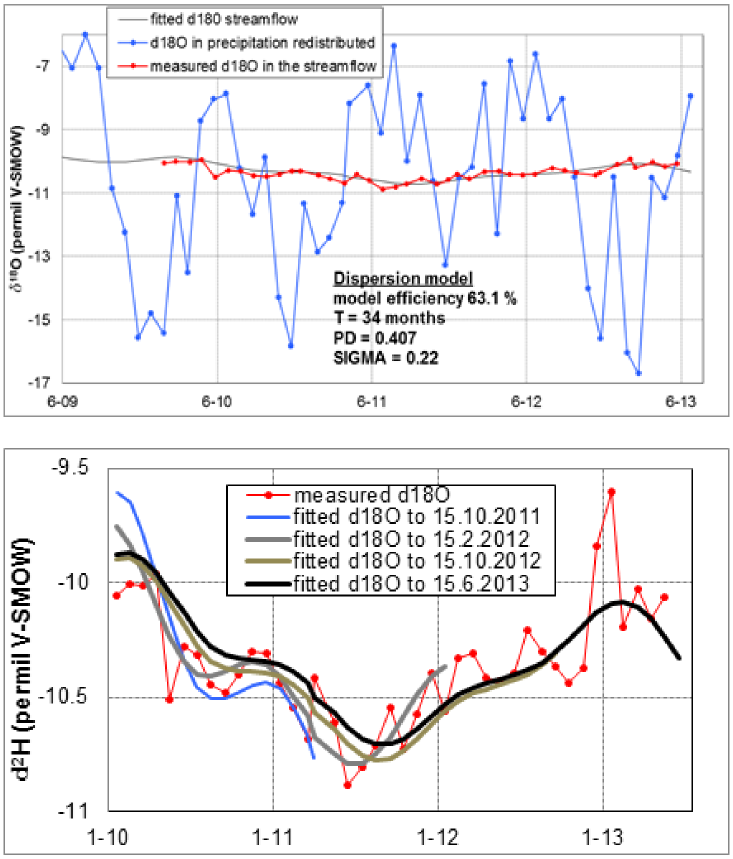


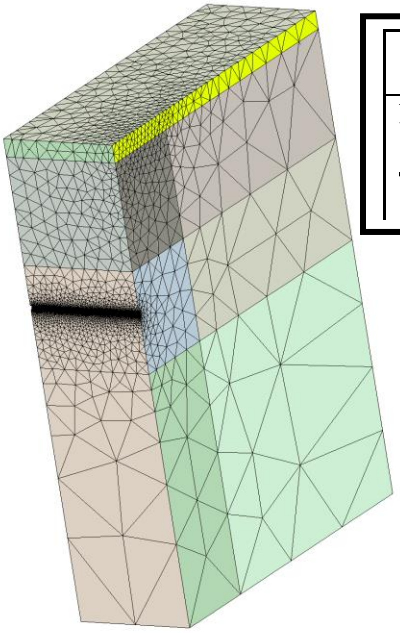
Figure 2-7: Results of water residence time (δ18O) of seepage site V7 calibrated by lumped parameter model (FLOWPC); (b) Estimations of water residence of δ^{18}O at seepage site V7 during extension of time series.

Table 2-2: Changes of parameters (bold numbers) at seepage site V7 during δ^{2}H, δ^{18}O time series of various lengths

	fitted to 15.10.11		fitted to 15.2.2012		fitted to 15.10.2012		fitted to 15.6.2013	
	d2H	d18O	d2H	d18O	d2H	d18O	d2H	d18O
Dispersion par.	0.2826	0.488	0.2735	0.5723	0.3557	0.3876	0.3632	0.407
Res.time [month]	**23.6**	**30.9**	**23.3**	**31.5**	**34.7**	**31.6**	**42**	**34**
Model effic [%]	80.3	80.1	72.1	73.5	71.6	68.1	60.1	63.1
SIGMA	0.224	0.027	0.252	0.028	0.155		0.143	0.22
Time of obs. [month]	20	20	24	24	32	32	40	40

2.2.5 Hydraulic model in 3D/2D

The model was constructed according to the definition, using the double planar symmetry – both sides of the fracture/fault plane and both sides of the tunnel. So only one half of the fracture/fault is considered in the model (Figures 2-8 to 2-9). The parameters and boundary conditions are given above in section 2.1. We calibrate the hydraulic conductivity of the deep 3D domain from the inflow from the rock continuum and the transmissivity of the 2D domain from inflow from the fracture or fault. The upper zone is chosen sufficiently permeable to keep approximately horizontal water table controlled by the boundary condition in the outer side of the model. The cases of recharge redistribution in the shallow permeable zone that explain the contrast of tunnel inflow and recharge between particular places are shown in Figure 2-10.



Number of	V7	V156	V2
Nodes	2431	16510	17229
Triangles	10964	10740	11355

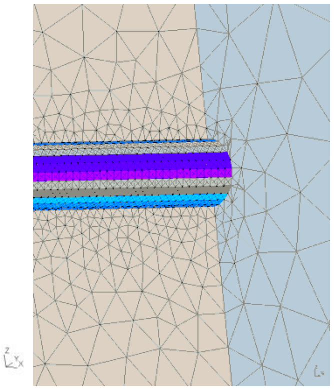


Figure 2-8: Examples of model meshes and their sizes for several cases differing by the tunnel depth

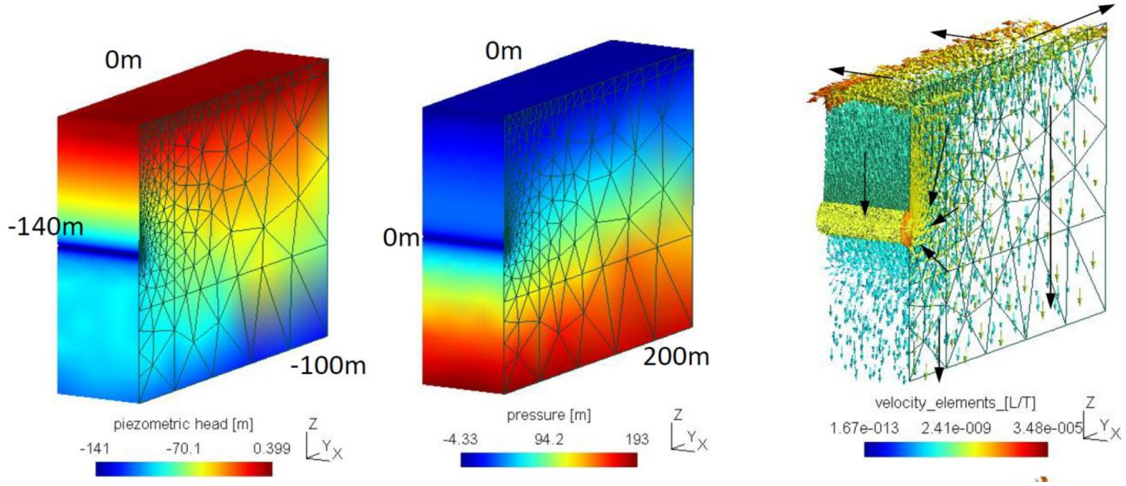


Figure 2-9: Demonstration of results – piezometric head, pressure and velocity fields

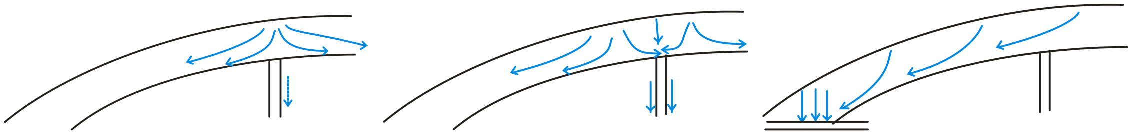


Figure 2-10: Cases of recharge redistribution in the shallow permeable zone, explaining contrast between the particular places of tunnel inflow and recharge for given model area

Table 1: Data of the fitted 3D models, three variants for different cases of measured inflow and residence time. Hydraulic properties and equivalent porosity are calibrated.

	Model 2 (V6)	Model 3 (V2)	Model 4 (V4)
tunnel depth [m]	-39	-140	-91
thickness of shallow zone [m]	-20	-15	-20
type of flow	shallow, weak	deep, weak	deep strong
type of 2D structure	single fract,	single fract,	fault zone
infiltration [mm/yr]	200	200	200
tunnel discharge (2D) [l/s]	0.01	0.00002	0.014
K shallow [m/s]	1.00E-06	1.00E-06	1.00E-06
K down [m/s]	5.48E-10	4.25E-12	5.63E-10
K fract [m/s]	1.15E-07	1.74E-06	3.22E-08
T fract [m^2/s]	1.15E-07	1.74E-10	1.61E-07
width of fault [m]	x	x	5
theroretical aperture [m]	5.50E-05	5.80E-06	x
width of 2D domain [m]	1	0.0001	
porosity	0.02	0.0001	0.0435
Mean res. time [months]	27.999	289	149.9
Mean res. time [years]	2.3	24.1	12.5

2.2.6 Transport model in 3D/2D

The model fitting process is such that we take the mean residence times estimated from lumped parameter models as “measurement” (i.e. given values) and calibrate the appropriate parameter of the model (provided the hydraulic parameters are already derived from water inflow rate), which is mobile water volume (i.e. porosity for equivalent continuum). For a special case of a single fracture, the hydraulic and transport properties are derived from a single parameter - aperture. So, the aperture (or porosity as a ratio of aperture to 2D domain width) is already given by the estimated transmissivity and the water velocity and residence time can be directly calculated. If this was applied on cases Model 2 (V6) and Model 3 (V2) (line “theoretical aperture” in Table 2-3), the predicted values of residence time were order of magnitude smaller than known from stable isotopes and tritium/helium. Therefore the interpretation that the flow is not through a single fracture is applied – we calibrate the porosity of equivalent layer of crushed rock or set of several fracture associated with selected 2D model thickness (1 m for clearness).

We checked some other features in the model how the tracer is split into parts, one flowing out of the model in the shallow permeable zone, the second sinking quickly to the vertical fracture and the third small part sinking in the 3D deep domain (less permeable) (Figure 2-12). We compare residence time evaluation methods, different characteristic points in breakthrough curves (Figure 2-11).

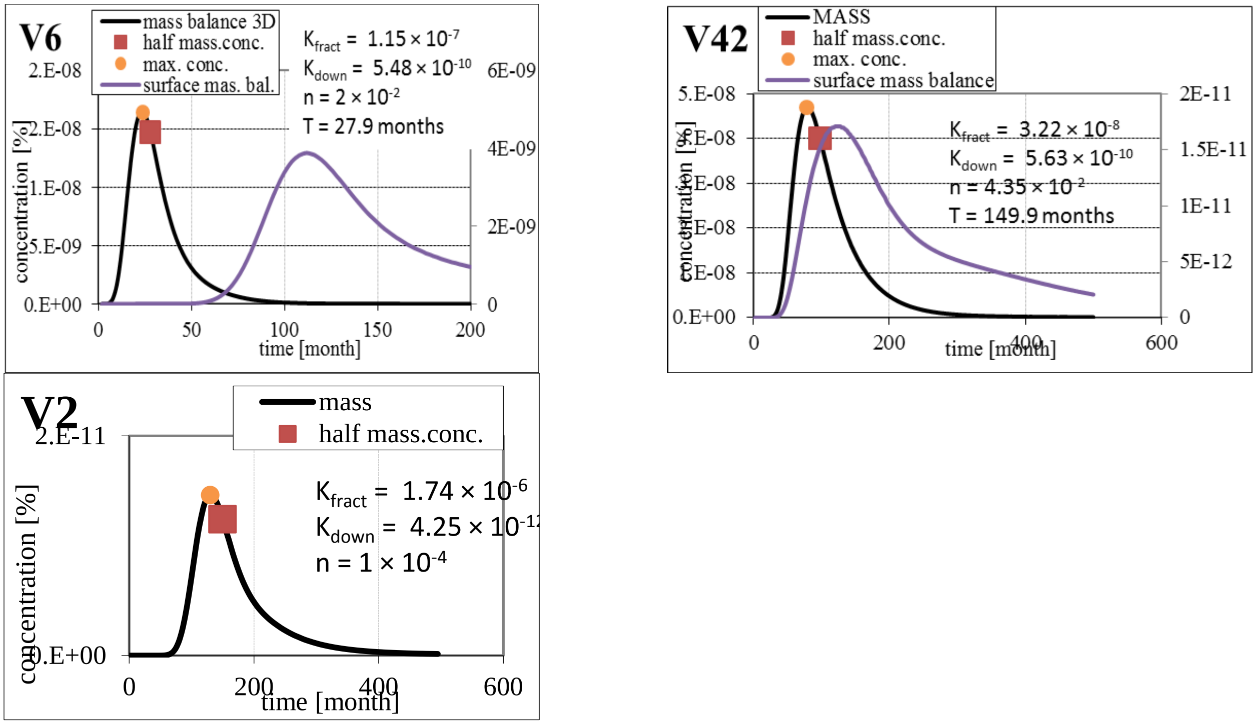


Figure 2-11: Breakthrough curves of fictitious tracer for three model variants corresponding to particular positions of inflow

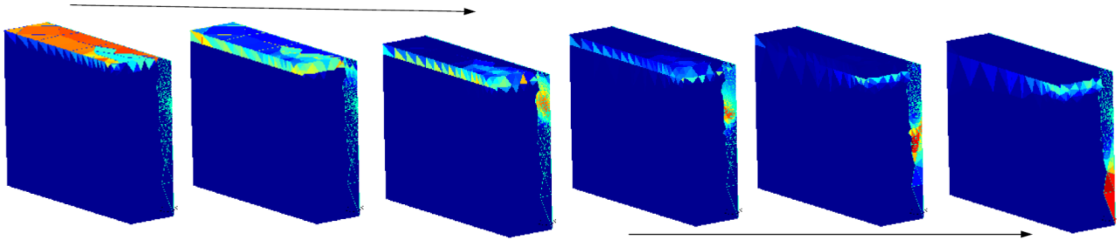


Figure 2-12: Time sequence of tracer distribution in the 3D domain and in the fracture

2.3 Contribution of BGR

2.3.1 Objectives of the BGR participation in Task C2

Since 1984 Federal Institute for Geosciences and Natural Resources (BGR), Germany has been involved in various experiments within the framework of German/Swiss collaboration at the Grimsel Test Site (Switzerland). The work are focused on the site characterisation covering flow in the fracture network (Liedtke et al. 1999), characterisation of tunnel near-field (Marschall et al. 1999), and flow and transport in the fracture system (Himmelsbach et al. 2003). Extensive know-how concerning rock characterization have been obtained and can be extended by involving in the Swedish investigation program in the underground laboratory Äspö since 1996.
A powerful numerical code based on the finite element method was continuously developed since 1986. The code (RockFlow), initially for simulating flow and solute transport in fracture network, was extended to a fully coupled thermal-hydraulic-mechanical-chemical code (OpenGeoSys – OGS). Validation of numerical model against experiments is an important issue for code development.

To keep and extend scientific and technological know-how, especially for the alternative rock formation in Germany, BGR is participating in the DECOVALEX-2015 Task C2 to analyze flow and transport processes in the granite massif around the Bedrichov tunnel (Czech).

2.3.2 Theoretical background and code used

The transient saturated groundwater flow is described by

$$S_0 \frac{\partial h}{\partial t} + \nabla \cdot v = q \, , \qquad (2\text{-}12)$$

where h is the piezometric head, S_0 is the specific storativity, v is the average fluid velocity vector, and q is the fluid sink/source.

The velocity is given by the three-dimensional, linear Darcy law:

$$v = -K \cdot \nabla h \, , \qquad (2\text{-}13a)$$

where K is the hydraulic conductivity tensor, or by the general form of various non-linear laws for fracture or tube flow:

$$v = -K^{*} \cdot (\nabla h)^{\alpha} \, , \qquad (2\text{-}13b)$$

where K^* is the hydraulic conductivity as a function of the piezometric head or its gradient and α is a coefficient for different non-linear flow laws (here $\alpha=1$ used).

If v is substituted into the mass balance equation (2-12), the equation may be rewritten as

$$S_0 \frac{\partial h}{\partial t} + \nabla \cdot (K \cdot \nabla h) = q \,, \tag{2-14}$$

which is the governing equation for the flow model.

The differential equation for solute transport is

$$\frac{\partial}{\partial t}(nc) + v \cdot \nabla c - \nabla (nD_s \cdot \nabla c) + n\lambda c + q(c - c^*) = 0 \,, \tag{2-15}$$

where *c* is the mass fraction of solute per fluid mass, *n* is the volumetric porosity, D_S is the diffusion/dispersion tensor, λ is the radioactive decay constant and c^* is the concentration of solute in the source fluid. This formulation includes dispersion effects according to Fick's first law. The three-dimensional diffusion/dispersion tensor in a ξ, η, ζ-coordinate system oriented according to the flow path is written as

$$D_s = \begin{bmatrix} \alpha_L |v| + d_0 & 0 & 0 \\ 0 & \alpha_T |v| + d_0 & 0 \\ 0 & 0 & \alpha_T |v| + d_0 \end{bmatrix}, \tag{2-16}$$

where α_L and α_T are the longitudinal and transverse coefficients of mechanical dispersion and d_0 is the diffusion coefficient. This is identical to the Scheidegger approach after transformation of D_s into a global x, y, z-coordinate system. The term $n\lambda c$ describes the non-conservative behavior of the solute and can be interpreted as a decay term for radioactive solutes, with λ for the decay constant in the decay law. The last term of equation (2-15) is the source term for fluid sources within the modelled domain. The abovementioned equations have been implemented in the code OGS.

2.3.3 Benchmarking exercises

Quality management is nowadays a standard tool for production and development to ensure a high quality of a produced result. A numerical code dealing with the coupled thermal-hydrologic-mechanical-chemical (THMC) processes is a highly complicated software product, since the different processes have different characteristic features, e.g. time and spatial scales, nonlinearities, and interaction degree etc. To keep the high quality of the developed code, benchmark testing is therefore necessary, especially when scientists from different disciplinary and different organization are working on the same code.

Before the code used for Task C2, benchmarking exercises have been performed for flow and transport problem. For the groundwater flow Theis' problem has been selected because there is a quasi-analytical solution (Kolditz et al. 2012).

The calculated drawdowns using different models (1D axially symmetric liquid model, 1D axially symmetric groundwater flow model and 2D groundwater flow model) as a function of time in the pumping point fit very well with the analytical solution (Figure 2-13-left). Similar verification exercise was done for the solute transport taking account of diffusion and sorption (Figure 2-13-right).

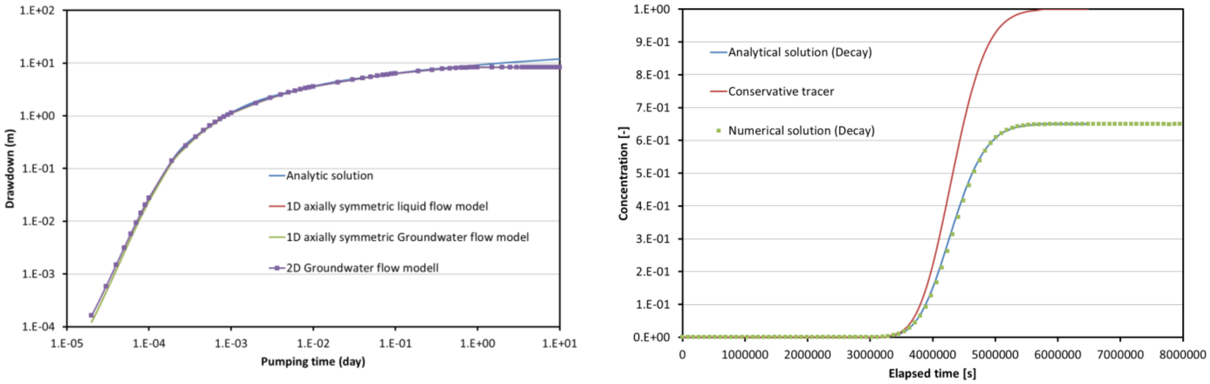


Figure 2-13: Model verification of groundwater flow (left) and solute transport (right)

2.3.4 Hydraulic models and results

The approach to understanding flow regimes in the Bedrichov tunnel is divided into two steps: (1) 2D single fault model at 1728 m and (2) 3D coupled fracture matrix model in all four sections selected as typical flow rate measured in the tunnel (Figure 2-3), based on the common task C2 definition (section 2-1). The 2D single fault model served as parameter estimation of main hydraulic properties. Comparison has been made using the data from 2007. The estimated parameter was used as calibrated values in the 3D coupled fracture matrix model for the consistency checking.

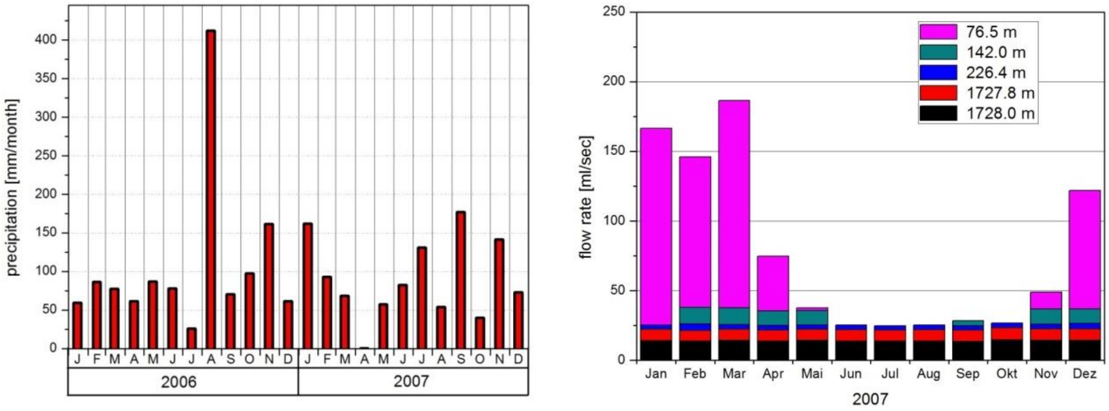


Figure 2-14: Measured precipitation (left) and flow rate in the tunnel sections (right)

Comparing the measured inflow rate in the tunnel and precipitation available for the year 2007, relative good correlation can be found with neglecting of freezing and melting of snow in the winter time. However, drought month (April) reflects on the tunnel inflow with one or two months delay (Figure 2-14). Considering a total attachment area in the observation area of 6.3 km^2, annual total water from precipitation in 2007 may be calculated to 6.8 million m^3. Total inflow water covering tunnel discharge at V-8 in the Bedrichov was however measured only by approx. 124000 m^3. This indicates that very small part (< 2%) of precipitation will contribute to the water inflow in the tunnel.

Based on the conceptual model (Fig. 2-1) a 2D single fracture model for the high permeable zone in the tunnel meter 1728 has been constructed for the hydraulic analysis (Figure 2-15). The model is assumed large enough to set no flow boundary condition at the bottom. Source term taking account of measured precipitation was considered at the top. Two different boundary conditions (both no flow and hydrostatic pressure) were used for variation. A fault model covering two zones (V-4/1 and V-4/2) with a thickness of about 0.2 m (distance between 1727.8 and 1728) was constructed.

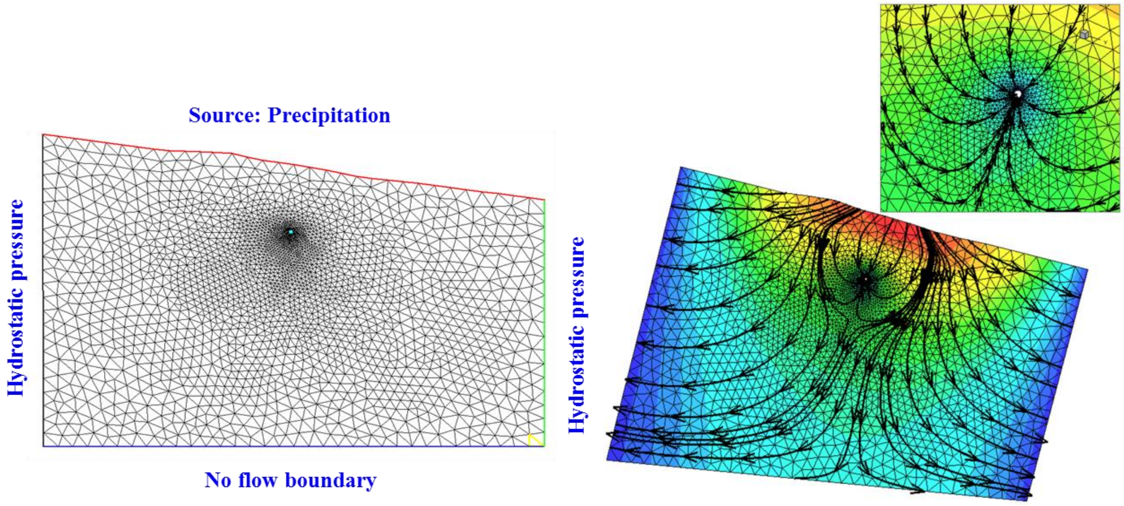


Figure 2-15: 2D single fracture model (left) and pressure distribution and flow path (right)

The 2D single fault model was considered as a homogeneous model with a basic dataset, in which the hydraulic conductivity was assumed to be 9.12×10^{-10} m/s and specific storage 1.3×10^{-6} /m. The basic dataset were calibrated by variation (Table 2-4). An additional variation taking account of a second domain with a higher permeability of about two orders of magnitude (hydraulic conductivity 9.12×10^{-8} m/s) in the upper part over the tunnel was carried out to analyze the water flowing time (Figure 2-16).

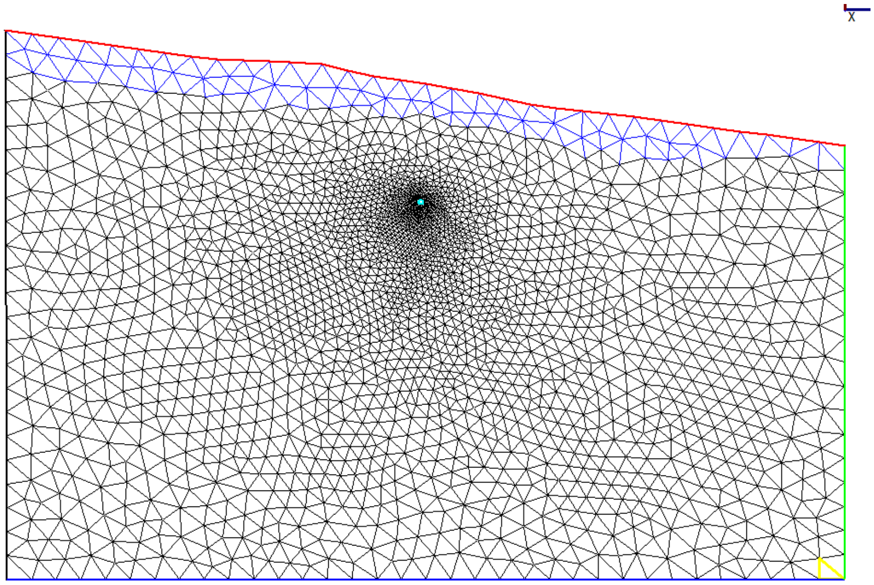


Figure 2-16: 2D single fracture model with 2 material groups

Table 2-4: Summary of cases/variations

Case/	Zone - 1		Zone - 2		Boundary condition	Precipitation	Constand inflow
variation	k (m/s)	S (/m)	k (m/s)	S (/m)		mm	m/s
1	9.12E-10	1.30E-07			hydrostatic	0	0
2	9.12E-10	1.30E-07			Constand	Seasonal curve	0
3	1.70E-06	1.30E-07			Constand	Seasonal curve X 15	0
4	2.50E-07	1.30E-05			Constand	Seasonal curve X 10	0
5	9.12E-10	1.30E-05			Constand	Seasonal curve	0
6	2.50E-07	1.30E-05			Constand	Seasonal curve	0
7	2.50E-07	1.30E-05			Constand	Seasonal curve X 12	0
8	9.12E-10	1.30E-06			Constand	Seasonal curve	0
9	9.12E-09	1.30E-06	9.12E-08	1.30E-06	hydrostatic	Seasonal curve	0
10	9.12E-09	1.30E-06	9.12E-08	1.30E-06	hydrostatic	Seasonal curve	3.00E-07

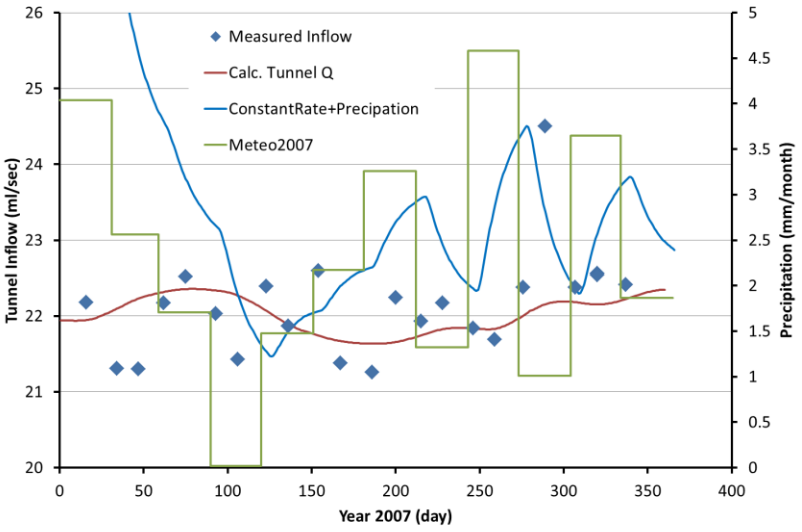


Figure 2-17: Measured and calculated inflow in the tunnel section 1728 as model calibration

As a result, only 20% of the tunnel inflow may directly be from the precipitation (Figure 2-17). About 80% of the inflow in the tunnel may come from a source with a constant flow rate about 18 ml/sec, which may be supposed from the neighbor reservoir due to a short distance between the considered tunnel section and the reservoir. The calculated flow path (Figure 2-15-right) should serve as a basis for the tracer transport analysis.

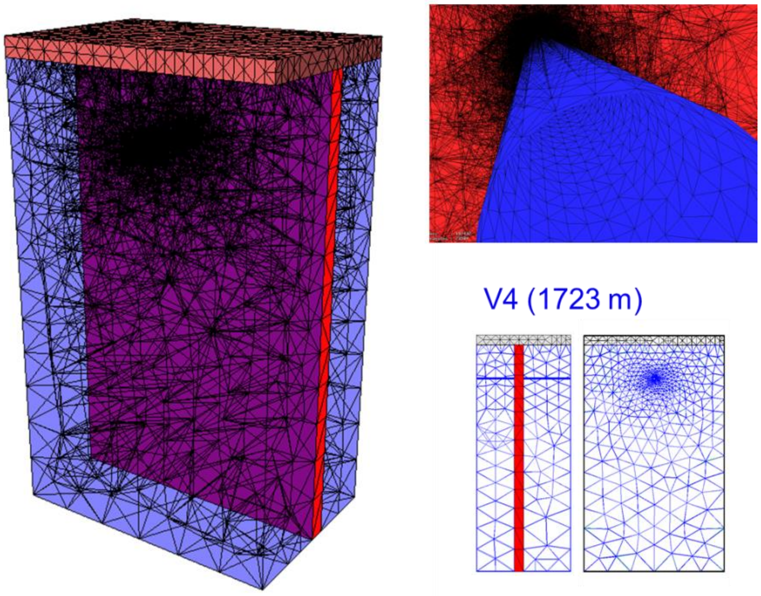


Figure 2-18: 3D fracture/matrix model

On the basis of the calibrated parameter from V-4, four 3D coupled fracture and matrix models (Figure 3) have been constructed to analyze the flow pattern in four different sections. Figure 2-18 shows an exemplary 3D mesh in the section of 1720 m with 67825 tetrahedral elements. Calculated total inflow fits quite well with the measured mean value (Figure 2-19). The Run1 is the calculations using the basic database with high permeability which fitted well with the trend of measured inflow data (seasonal effect). The Run 2 is the results with a reduction of permeability of one order of magnitude for both fracture and matrix zones.

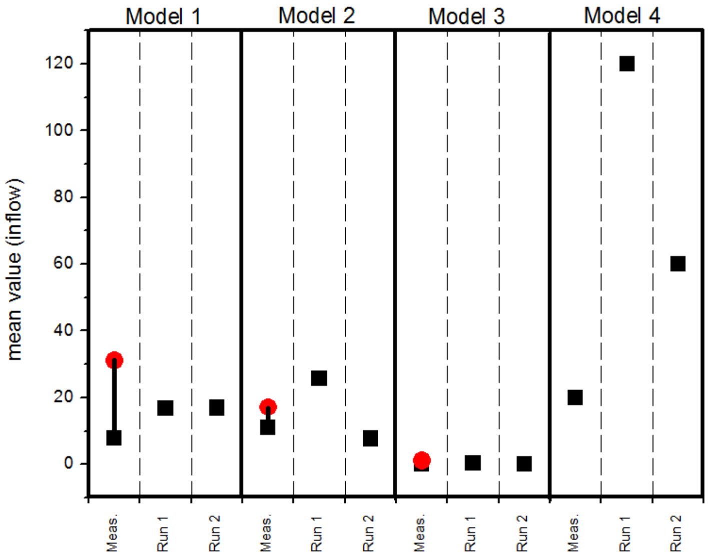


Figure 2-19: Tunnel inflow analysed by four 3D models (min and max during time is shown as measurement)

Generally fault zone/fracture with high permeability, sometimes several orders of magnitude higher than those of rock mass assumed 4 OOM in our model, dominates the flow regime. The rock mass has only a storage effect due to its huge volume. This difference in permeability brings some numerical convergence problems. Otherwise, the full 3D model requires long calculation times. Based on the updated information on the four 3D models during the Mont Terri Workshop (Nov. 2013), new calculations will be done for the comparison with other teams. Documented isotope data will be analyzed and prepared for the transport calculation based on the flow path analysis from the flow model.

2.4 Contribution of DOE-UFD (Sandia)

2.4.1 Lumped Parameter Modeling

The concentration of a tracer a sampling point is a function of the distribution of groundwater age ($g(\tau)$) given by the convolution integral:

$$C(t) = \int_0^\infty C_{in}(t-\tau)g(\tau)e^{-\lambda t}d\tau \tag{2-17}$$

where C_{in} is the input function for the tracer and λ is the decay constant for the tracer of interest. Age distributions have been developed for a variety of simple aquifer type and flow systems (e.g. Cook, 2000). The models used in this study include commonly used dispersion and exponential model as well as a newly developed model which includes matrix diffusion in fractured systems. For the exponential model:

$$g(\tau) = \frac{1}{\tau}e^{-\frac{t-\tau}{\tau}}\ , \tag{2-18}$$

and for the dispersion model:

$$g(\tau) = \left(\frac{4\pi(t-\tau)^3}{Pe\tau}\right)^{1/2} exp\left(-1-\frac{t-\tau}{\tau}\right)^{2\tau Pe(t-\tau)}\ , \tag{2-19}$$

where Pe is the peclet number for transport. In order to account for matrix diffusion we use the random walk in time method after Painter (2008). Here the retarded travel time distribution is given by:

$$g(t_{tr}) = \int_0^\infty \int_0^\infty g_{ret}(t_{tr}-\tau|\beta)g_{\beta|\tau}(\beta|\tau)g(\tau)d\tau d\beta \tag{2-20}$$

where τ is the non-retarded advective travel time, β is the transport resistance parameter and t_{tr} is the total travel time include retention. The retention time distribution can be derived for a variety of processes including unlimited matrix diffusion which is given by (Painter, 2008):

$$g_{ret} = H(t_{ret})\kappa\beta/2\sqrt{\pi t_{ret}}exp(-\kappa^2\beta^2/4t_{ret}), \tag{2-21}$$

where:

$$\kappa = \theta_{im}\sqrt{DR_{im}} \tag{2-22}$$

is a function of the immobile porosity θ_{im}, effective diffusion coefficient and immobile retardation factor R_{im}. We incorporate matrix diffusion via the random walk in time methodology after Painter (2008) by sampling an advective travel from travel time distributions of a dispersive and exponential age distribution, then sample the resistance parameter given the travel time, then sample from the retention time distribution give the resistance parameter to calculate a total travel time. The total travel time distribution is then reconstructed from these samples.

Observations of isotopes at the Bedrichov tunnel were then used to constrain the mean age of the lumped parameter models. For a given conceptual model, lumped parameter models were run with different mean groundwater age (τ) and the resulting modeled isotope concentrations compared with observed concentrations.

2.4.2 Hydraulic Modeling with PFloTran

In this study we use PFLOTRAN, a scalable, parallel, multi-phase, multi-component, non-isothermal reactive flow and transport code to simulate multiple environmental tracer concentrations in heterogeneous 2-D and 3-D domains. For all simulations in this paper PFLOTRAN was run in the Richard's equation mode, which simulates variably saturated single phase flow and transport.
The mass balance equation for Richard's flow solved by PFLOTRAN is given by (Hammond et al 2012):

$$\frac{\partial}{\partial t}(\phi s q) - \bigtriangledown \cdot (\rho q) = Q_w \qquad (2\text{-}23)$$

where Q_w is the total water discharge, φ is the porosity, s is the water saturation, ρ is the water density and q is the Darcy flux is given by (Hammond et al 2012):

$$q = -\frac{k k_r}{\mu} \bigtriangledown \cdot (p - \rho g z) \qquad (2\text{-}24)$$

where k is the intrinsic permeability, k_r is the relative permeability, μ is the viscosity and g is the acceleration of gravity. The multi-component, multi-phase geochemical mass conservation equation is written (Hammond et al 2012):

$$\frac{\partial}{\partial t}\left(\phi \sum_{\alpha} s_\alpha \Psi_j^\alpha\right) + \bigtriangledown \cdot \sum_{\alpha} (q_\alpha - \phi s_\alpha D_\alpha \bigtriangledown) \Psi_j^\alpha = Q_i - \sum_m v_{jm} I_m - \frac{\partial S_j}{\partial t} \qquad (2\text{-}25)$$

where the sum is over α fluid phases, D_α is the dispersivity tensor, Q_j is a generic source or sink term, the sum $\sum_m v_{jm} I_m$ represents the sum over all mineral reactions with stoichiometric coefficient v_{jm} and mineral reaction rate I_m and S_j is the concentration of sorbed species. Ψ_j^α is the total concentration in the α fluid phase for the primary species given by (Hammond et al 2012):

$$\Psi_j^\alpha = \delta_{l\alpha} C_i^l + \sum_{i=1}^{N_L} v_{ij} C_i^\alpha \qquad (2\text{-}26)$$

where the l subscript denotes the liquid phase C_j^l are the primary species v_{ji} are the stoichiometeric coefficients relating the primary species to the secondary species C_i^α. The secondary species are calculated by (Hammond et al 2012):

$$C_i^\alpha = (\gamma_i^\alpha)^{-1} K_i^\alpha \prod_{i=1}^{N_L} (\gamma_i^l C_i^l)^{v_{ij}} \qquad (2\text{-}27)$$

with equilibrium constant $K_i^\alpha$and activity coefficient γ_i^α and γ_j^l.

PFLOTRAN solves Equations (1)-(5) using fully implicit, integral finite volume. PFLOTRAN is written in object oriented FORTRAN 9X and uses Message Passing Interface for distributed-memory, domain-decomposition parallelism. The Portable Extensible Toolkit for Scientific Computation (PETSc) library is leveraged to provide access to cutting edge parallel Newton-Krylov solvers. Parallel IO is achieved using the HDF5 file format. PFLOTRAN is written to be employed on a variety of architectures and scales from single processor laptops to 2^{17} core petascale simulations (Hammond et al 2012).

2.4.3 Lumped Parameter Results

Modelled stable δD composition in the Bedrichov tunnel at sampling point V6 for an exponential age distribution with mean ages of 1, 2.5, 5 and 10 years is show in Figure 2-20. The exponential model is incapable of fitting the observed data for any age distribution and shows a bias toward heavy isotopes. Models stable δD composition in the Bedrichov tunnel at sampling point V6 for a dispersion age distribution with mean ages of 1, 2.5, 5 and 10 years is shown Figure 2-20. The dispersion model fits the observed data slightly better, but as in the case of the exponential model, the dispersion model produces consistently heavy isotopic signals for all ages modelled. A similar bias in modelled results was observed for all other sample locations. This bias is an effect of preferential seasonal recharge of winter snow melt – as can be observed in Figure 2-20. Future work will include developing a seasonally weighted input function.

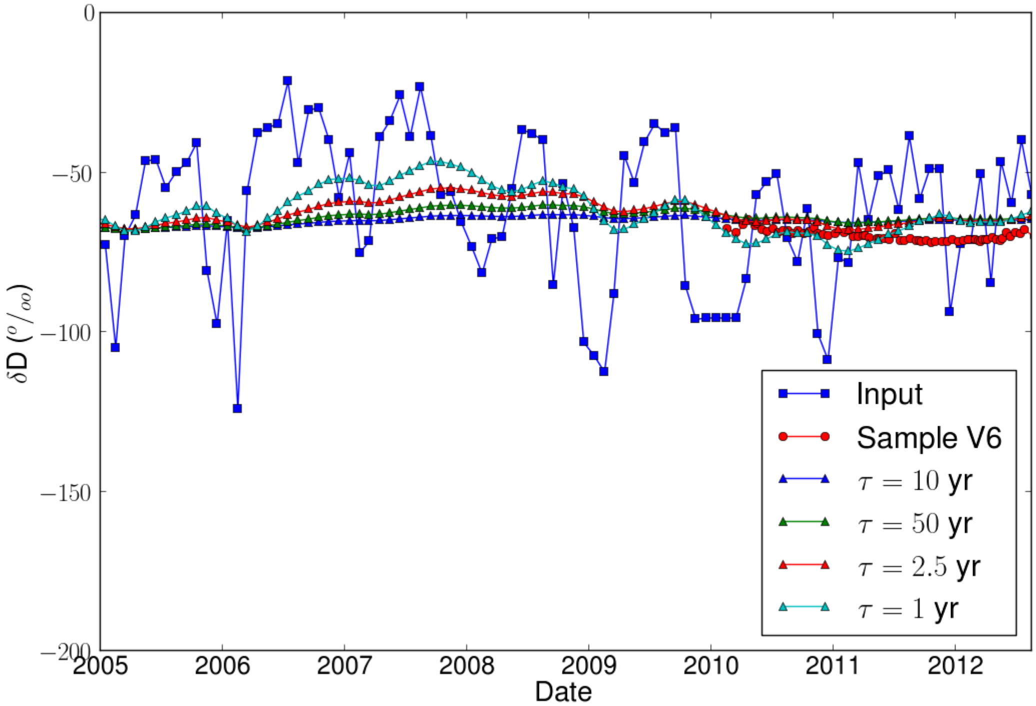


Figure 2-20: Measured and modeled stable isotope composition for the Bedrichov collection canal using the exponential age distribution

A tracer plot of tritium versus CFC-12 is shown in Figure 2-21. Tritium in Bedrichov precipitation was created using an inverse distance weighted average of surrounding records including Vienna, Prague, and Uhlirska. Given the close proximity of the site to Uhlirska, the input function is very close to that dataset during years with data. The expected concentration measured in 2012 for increasing mean age is plotted in the dashed red line. Black dots indicate 5 year intervals in mean age. From Figure 2-21, it is apparent that waters discharging the Bedrichov tunnel are generally less than 5 years in age. This is the case regardless of the age distribution chosen. Thus, we conclude that fluid flow in the Bedrichov fractures rapid and groundwater ages are less 5 years for almost all samples.

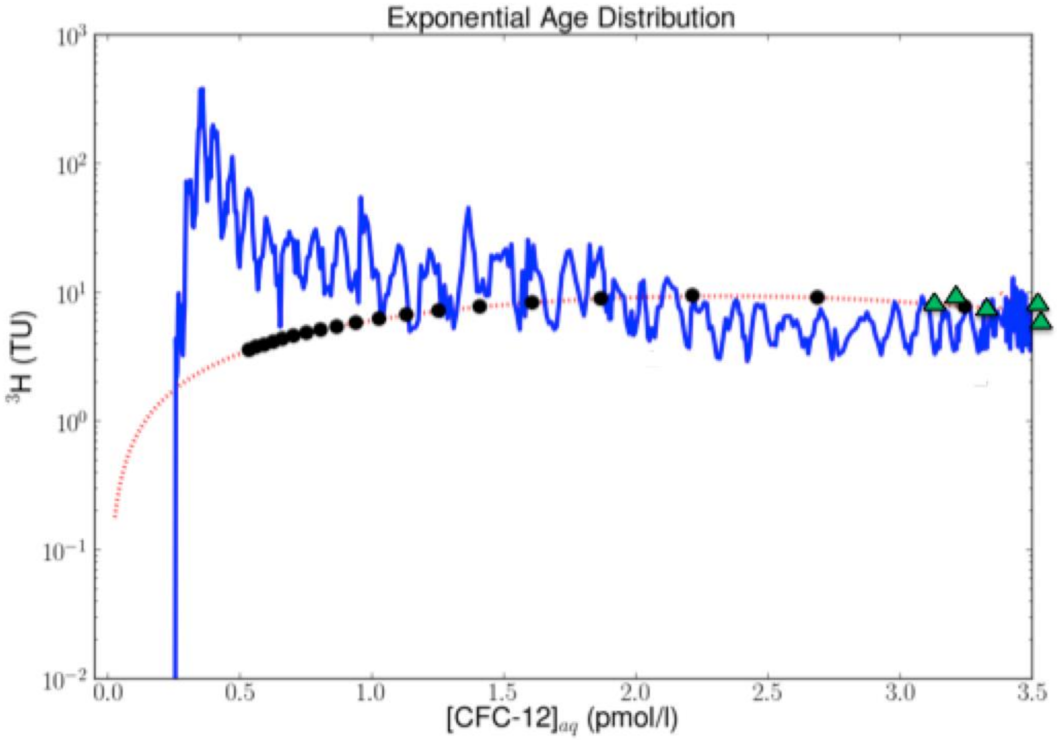


Figure 2-21: Tracer plot of 3H vs CFC-12 for precipitation (blue line) at Bedrichov, measured samples (green triangles) and expected concentration for the year 2012 given an expontial age distribution as a function of increasing mean age. Black circles are the expected concentration for every 5 year interval of mean age.

We explored the effect of matrix diffusion at the Bedrichov site using our random walk in time method. Figure 2-22 shows the expected travel times for dispersion only and for dispersion and retention assuming infinite matrix diffusion. Here we assume matrix diffusion parameters representative of the Bedrichov site, and assign a mean advective travel time was 2 years, matrix porosity of 1% and fracture diameter of 0.2 mm. We observe no difference in the age distribution in Figure 2-22 and find that the mean total travel time including retention is indistinguishable from the mean travel time considering advection alone. Figure 2-23 shows the advective and total travel time distributions for a system with a mean advective travel time of 100 years, 10% matrix porosity and fracture width of 0.2 mm. There is a clear effect of matrix diffusion in Figure 2-23 and the mean total travel time of 5000 years is significantly different than that of purely advection alone.

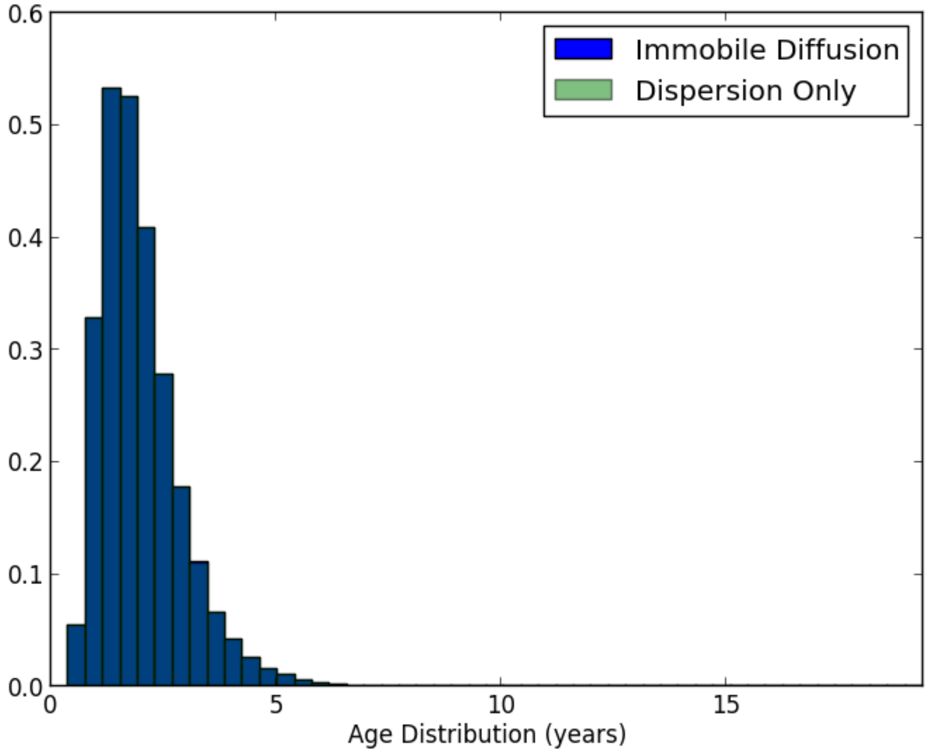


Figure 2-22: Expected age distributions for a dispersion model only and a dispersion model which includes retention time from infinite matrix diffusion for a mean advective travel time of 2 years, a matrix porosity of 1% and a fracture diameter of 0.2mm. (For these parameters, the age distributions are identical.)

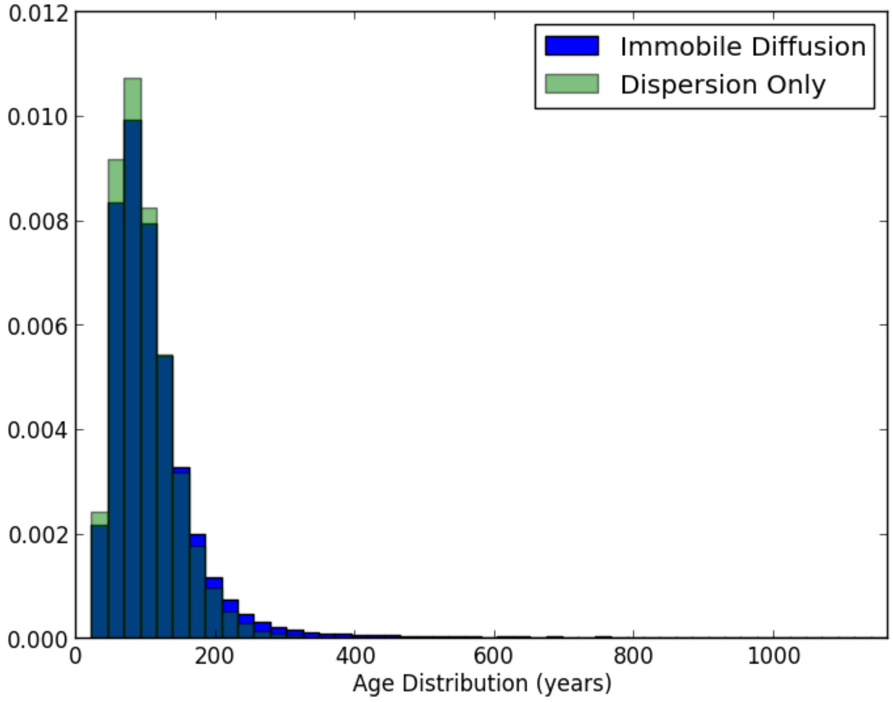


Figure 2-23: Expected age distributions for a dispersion model only and a dispersion model which includes retention time from infinite matrix diffusion for a mean advective travel time of 100 years, a matrix porosity of 10% and a fracture diameter of 0.2mm.

2.4.4 Hydraulic Model Results

For increased accuracy using PFLOTRAN's integral finite volume technique, unstructured, quadrilateral meshes for each conceptual model were constructed using the CUBIT meshing software. An example of a resulting mesh is given in Figure 2-24. A summary of all mesh sizes for conceptual models 2-4 is given in Table 2-5.

Table 2-5: Summary of mesh sizes for the models run

	V1,V5,V6	V2	V4
Elements	84656	73684	89284
Nodes	90630	79182	95506

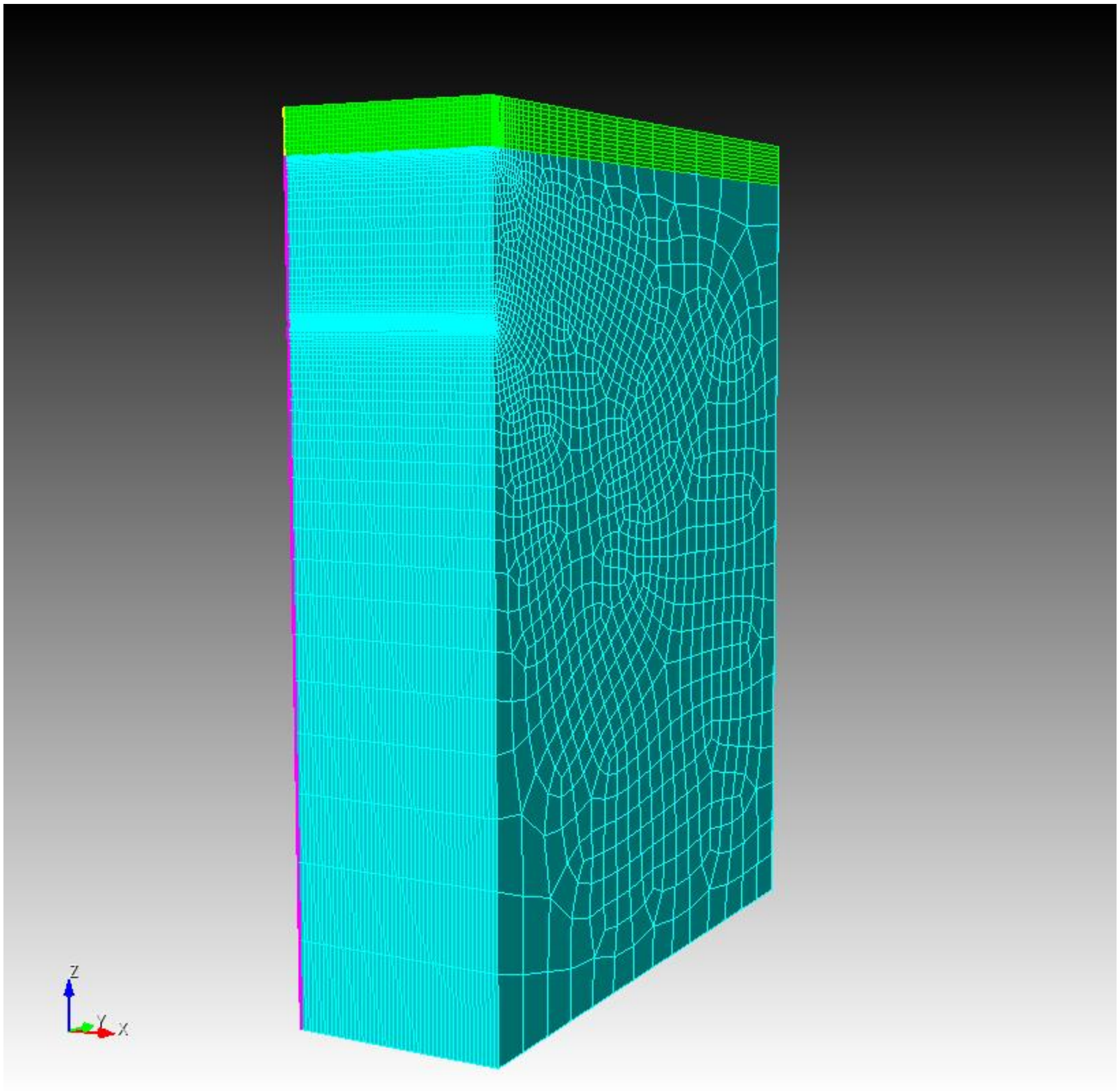


Figure 2-24: Example mesh for conceptual model 4. Total mesh elements ~ 90K, nodes ~ 96 K

Boundary conditions for the model were assigned according to the conceptual model described above. Simulations were run for a suitable period of time to achieve steady state conditions. An example of the flow solution is shown in Figure 2-25 for the V2 simulation at steady state. The steady state head distribution appears to be reasonable.

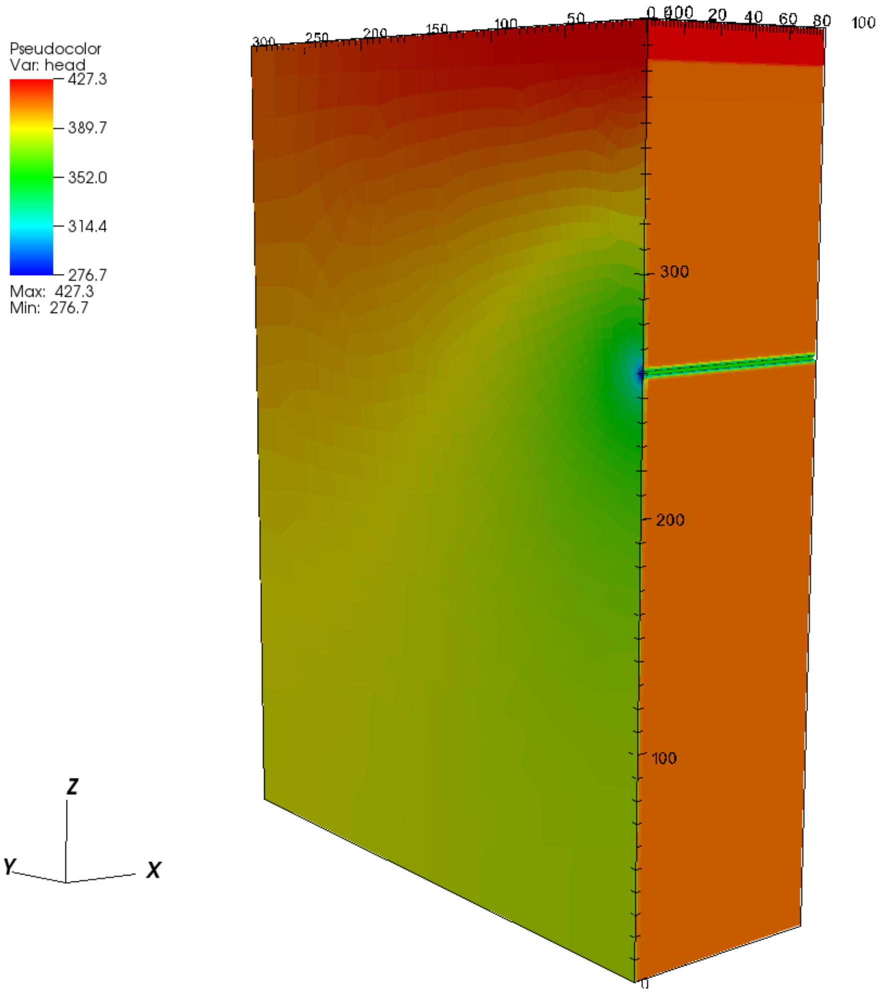


Figure 2-25: Steady state head distribution for the V2 simulation

Fracture zone permeability was calculated by matching the steady tunnel discharge to the appropriate value given in task description. Results for all conceptual models are summarized in Table 2-6. An example of a time series of solute transport in the V5 simulation is given in Figure 2-26. The observed breakthrough in the tunnel is given in Figure 2-27.

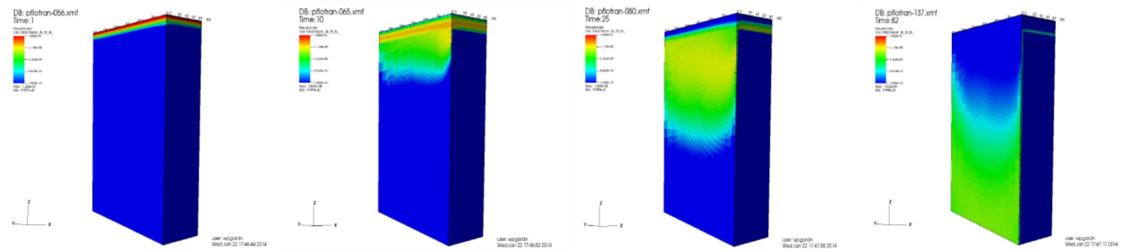


Figure 2-26: Transport sequence of tracer for the V5 simulation. Note that tracer concentration is contoured in log scale. Fracture plane on left side of domain, tunnel on right (front) of domain.

Table 2-6: Sandia Results summary

Model	Model 2 V1	Model 2 V5	Model 2 V6	Model 3 V2	Model 4 V4
tunnel depth (m)	-39	-39	-39	-140	-91
Shallow zone thickness (m)	-20	-20	-20	-15	-20
type of flow	shallow, weak	shallow, weak	shallow, strong	deep, weak	deep, strong
Type of 2D structure	single fract	single fract	single fract	single fract	fault zone
recharge (mm/yr)	200	200	200	200	200
tunnel discharge 2D (ml/s)	0.02	3	10	0.02	20
K Shallow (m/s)	1.0E-06	1.0E-06	1.0E-06	1.0E-06	1.0E-06
K Deep (m/s)	1E-15	1E-15	1E-15	1E-15	1E-15
k fract (m^2)	5E-17	5E-15	2E-14	2E-17	2.5E-14
K Fract (m/s)	4.9E-10	4.9E-08	2.0E-07	2.0E-10	2.5E-07
T Fract (m^2/s)	4.9E-10	4.9E-08	2.0E-07	2.0E-10	2.5E-07
Width of Fault (m)	x	x	x	x	1
Theoretical Aperature (m)	8.43E-06	3.91E-05	6.21E-05	6.21E-06	x
Width of 2D domain	1m	1m	1m	1m	1m
porosity	8.43E-06	3.91E-05	6.21E-05	6.21E-06	0.1
Mean res. Time (months)	2064	240	180	91524	102
Mean res. Time (yrs)	172	20	15	7627	9

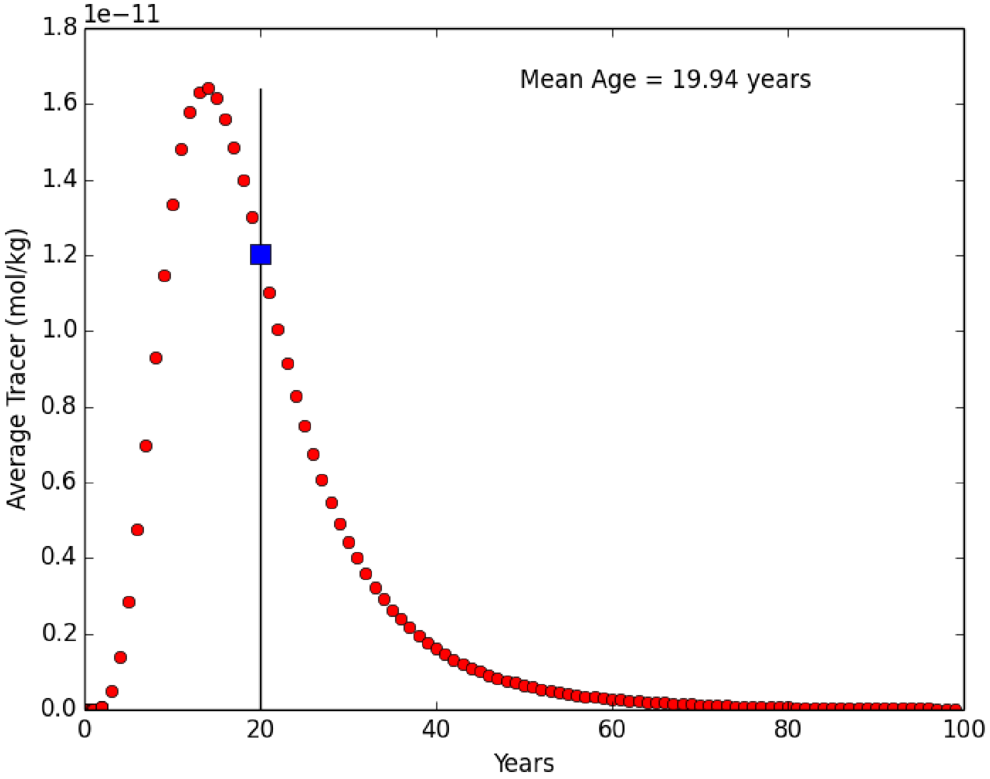


Figure 2-27: Concentration breakthrough in the tunnel and calculated mean age from the breakthrough for the V5 simulation. This plot is for total tunnel discharge.

2.5 Synthesis of approaches and results

The solution of all three teams presented in this report represents an introductory phase of work on Task C2. The common point is a solution of steady-state model problems of tunnel inflow, for four cases of different depth and different configuration of compact rock domain, fracture/fault plane, and shallow permeable zone. Each team had also some extension either aiming to the next phase (unsteady case of flow, tracer transport) or helping to understand the problem and given data (similar alternative model problems of BGR).

All teams were able to follow the suggested concept of combining 3D domain of rock matrix or equivalent continuum and 2D domain representing a fracture or fault zone. The software PFLOTRAN (of Sandia) and OpenGeoSys (of BGR) are based on standard finite elements while FLOW123D (of TUL) is based in mixed finite elements. All uses meshes of similar size in tens thousand elements (tetrahedra).

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Resulting calibrated conductivities are partly different between the teams, which is result of different selection of fixed and calibrated parameters. Basically the understanding of problem is same and the problems could result same with exactly same input. It will be settled in the next period. There are more differences between tracer transport solution of TUL and Sandia. The residence time differs by orders of magnitude with compatible hydraulic parameters and porosity. Based on discussion we explain it as an effect of matrix diffusion which is considered by Sandia but ignored by TUL. On the other hand the TUL values (porosity/aperture together with residence time data) appear more realistic taking into account data of natural tracer lumped parameter models. The solution in the next period will be concentrated on transient effects of infiltration – from groundwater table in the shallow zone to the tunnel inflow from fractures/fault zones.

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3. UFD-KAERI Collaboration on Development of Site Characterization Techniques for Fractured Crystalline Rocks

The U.S. Department of Energy Office of Nuclear Energy, Office of Fuel Cycle Technology established the Used Fuel Disposition Campaign (UFDC) to conduct the research and development (R&D) activities related to storage, transportation and disposal of used nuclear fuel and high level nuclear waste. The UFDC is currently evaluating the viability of mined repositories in various geologic media (i.e., salt, clay, granite) as well as deep borehole disposal in crystalline rocks. The UFDC R&D activities focus on general tool development, generic data collection, and enhanced understanding of geologic media and processes involved in waste disposal through integrated modeling, laboratory and field work (Wang, 2013). Given the genric nature of the work, the models and methods for improved understanding will be developed without site-specific data from an actual site considered for disposal in the U.S. Data from representative geologic environments (salt, clay/argillites/shale, and crystalline rock) obtained through international collaboration and literature searches can potentially be used for the generic R&D, to ensure that the models and methods work for the desired purpose.

Korea Atomic Energy Research Institute (KAERI) has engaged, on behalf of the Used Fuel Disposition Campaign (UFDC) - the Sandia National Laboratories (SNL), to conduct three collaborative tasks to support the study of high-level nuclear waste disposal in crystalline geologic media: (1) sharing KURT site characterization data, (2) technique development for in-situ borehole characterization, and (3) streaming potential (SP) testing. The first task was completed in FY13 (Wang et al., 2013). The work for FY14 has been focused on Tasks 2 and 3. This section summarizes the progress that has been made for these two tasks.

3.1 Roadmap for the Technique Development and Demonstration for In-situ Borehole Measurement

This subsection is a deliverable for the task 2 - technique development for in-situ borehole characterization. In this task, KAERI and SNL intend to develop a roadmap for the technique development and demonstration for in-situ borehole measurements. Key techniques are identified and the preliminary demonstration will be initiated using the DB-2 borehole.

3.1.1 Overview of KURT (KAERI Underground Research Tunnel)

To maintain the sustainability of atomic energy, the development of a radioactive waste disposal system is indispensible. To develop the reference high-level waste (HLW) disposal system the has carried out a long-term basic research and technology development program for the direct geological disposal of spent nuclear fuel since 1997 and proposed a preliminary disposal concept in 2002 (Figure 3-1). The R&D program funded by the Ministry of Science and Technology (MOST) with support from academic institutes and national research organizations involved a number of activities, i.e., repository system development and performance/safety assessment, a nuclide migration study and a geoscientific study. These activities were organized to achieve the common objective, i.e., the development of a Korean reference disposal system for high-level waste. As the main outputs from the HLW disposal study for past 10 years, KAERI presented the results of the performance safety of the disposal concept and the Korean reference disposal system in 2006, which has been proven adequate for the given geological characteristics in Korea. To investigate the feasibility, stability and safety of the proposed disposal concept, it is necessary to experimentally investigate the disposal system under an underground condition.

KAERI has also focused on the processes suitable for reducing the volume of spent nuclear fuel and recycling valuable fissile materials. The promising technologies developed by KAERI include the pyroprocessing of spent nuclear fuel and a geological disposal system of HLW. Accordingly, since 2007, KAERI has been leading an R&D program for recycling spent nuclear fuel, as well as a geological disposal system for HLW from the pyroprocessing stage. The core of the KAERI study was to characterize the geological media, design a repository system, and assess the safety of the disposal system (KAERI, 2011).

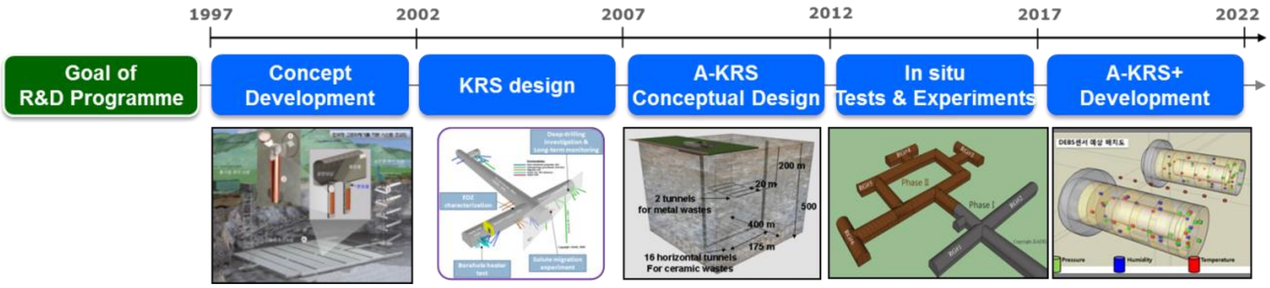


Figure 3-1. History of HWL R&D program in Korea

KURT is an underground research laboratory that intends to obtain information on the geological environment and behavior and performance of engineered barriers under repository conditions. The Planning Committee for the Korean Nuclear Energy R&D Program decided to construct a small-scale underground research laboratory at KAERI to test the proposed HLW disposal concept in 2003. Site characterization and a detailed design for the construction of KURT were completed in 2004. The design requirements for KURT were as follows (Cho et al., 2008):

1. The long-term stability of the tunnel should be ensured with minimum rock support.
2. Damage to the host rock from an excavation should be minimized.
3. The access tunnel should be linear to obtain the maximum overburden of the research modules with the minimum length of the access tunnel.
4. The research modules should be located at the rock mass with good quality.
5. The research modules should be located in a fresh bed rock with the minimum thickness of 50 m.
6. Construction should be economical as possible.

In November 2004, KAERI received a construction license from the municipal local governments of Daejeon city and Yuseong district, as well as from the Ministry of Science and Technology (MOST). Construction of Phase I of KURT started in March 2005 and was completed in November 2006.

The drilling and blasting method was applied to make a horseshoe shaped access tunnel and research modules. A careful blasting to minimize the blasting impact on the research reactor and other neighboring buildings at KAERI was required. Daily excavation was advanced about 1–3 m depending on the rock quality. The tunnel was supported mainly by using rock bolts and shotcrete in some zones of the tunnel. Lattice girders were installed at weak zones around the tunnel entrance and the fracture zones (Cho et al., 2008).

KURT has a total length of 255 m with a 180 m long access tunnel and two research modules with a total length of 75 m. The maximum depth of the tunnel is 90-100 m from the peak of a mountain that locates over the site. The horseshoe-shaped tunnel section is 6 m wide and 6 m high (Figure 3-2). The Phase II expansion of the tunnel is currently on its way and expected to be completed in November 2014. The host rock is granite, which is one of the potential host rock types for an HLW disposal repository in Korea. The utilization of radioactive material in KURT is not allowed.

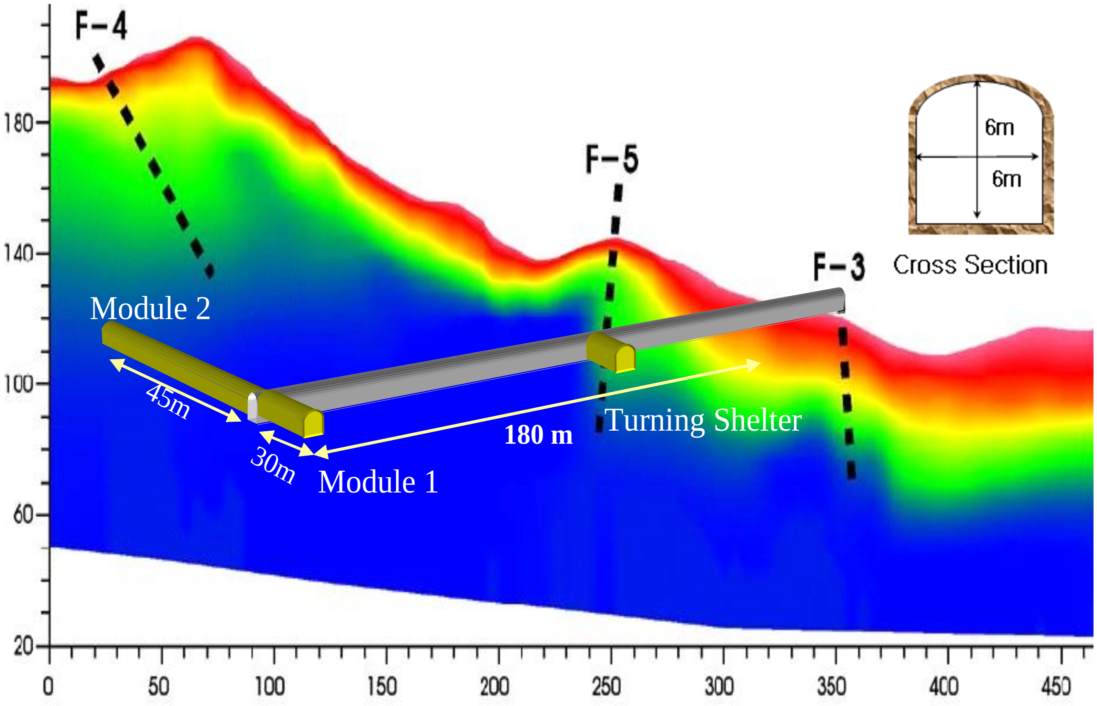


Figure 3-2. Current layout of the KURT

The main objectives of the KURT project are

1. To obtain information on the geologic environment, and the behavior and performance of engineered barriers under repository conditions
2. To establish the techniques for site investigation, data analysis and integrated assessment of the deep geological environment
3. To develop and demonstrate the proposed disposal concept and the technologies needed for the construction, operation and closure of a repository.
4. Public relations : information center for public and stakeholders.

Data collected from geological investigations provide important information for the design and safety assessment of a repository system. Various geological investigations at the KURT site have been progressed, including developing site descriptive models and collecting geological, hydrological, and geochemical baseline datasets.

KURT has also played a significant role in developing and demonstrating a repository disposal system as well as the technologies needed for its construction and closure. The research experience gained at KURT has provided important information to validate the safety and feasibility of a disposal system and has made important contributions toward the successful implementation of a future commercial geological repository program.

3.1.2 Geology of the KURT site

The KURT is located in KAERI, which is stationed in the Yuseong area and occupies the northem part of the city of Daejeon, Korea. The Yuseong area is approximately 150 km south from Seoul and belongs to the Keum River drainage basin in the western part of the Korean peninsula. The topography of the area is characterized as having fairly rolling hills surrounded by upland with elevations of 300- 500 m. The highest point in the distant area was about 850 m, and most of the lowlands were located at an elevation of approximately 50 m. The geology of the Yuseong area is composed of Precambrian metamorphic and Mesozoic plutonic rocks and dikes (Figure 3-3). The Precambrian metamorphic rocks are distributed in the northwestern part of the study area and composed mainly of biotite gneisses and schists. They are intruded widely by plutonic rocks. The gneisses and schists are gradationally related. The Mesozoic plutonic rocks are composed of schistose granite, biotite granite, two-mica granite, and dike rocks. The two-mica granite is distributed most widely in the Yuseong area (Ryu, 2012).

Two-mica granite with discernible foliation is a major rock type in cored rock samples at the KURT site. Under the microscopic observation of dri11 cores, the two mica granite consists mainly of quartz, plagioclase, orthoclase, biotite, and muscovite, along with small amounts of chlorite, rutile, zircon, and apatite as accessory minerals. The two-mica granite often showed as biotitic granite and schistose biotitic granite in some biotite-concentrated areas. Sericitization is commonly observed along the twin or grain boundaries of the plagioclase, and chloritization is seen along the cleavages in the biotite. Some iron oxides exist as a glassy vein along the micro-fractures. The results of the modal analysis from fresh host rocks collected from the deep boreholes (YS-1 and DB-1) illustrate the existence of a classified table of plutonic rock, which is mostly distributed in the granite region. The plagioclase of the fresh two-mica granite has an albite to oligoclase composition, and the biotite has an Al-depleted composition.

Whole-rock analyses of the major and trace elements suggest that the two mica granite is I-type and peraluminous granite and was formed by a differentiation of the calc-alkaline series. The SiO_2 content varies from 66.4 to 75.0%. The contents of TiO_2, $A1_2O_3$, MgO, FeO_T , CaO, and P_2O_5 tend to have negative correlations with SiO_2, whereas K_2O has a positive correlation with SiO_2, which are the usual tendencies of granite (Kim et. al., 2004).

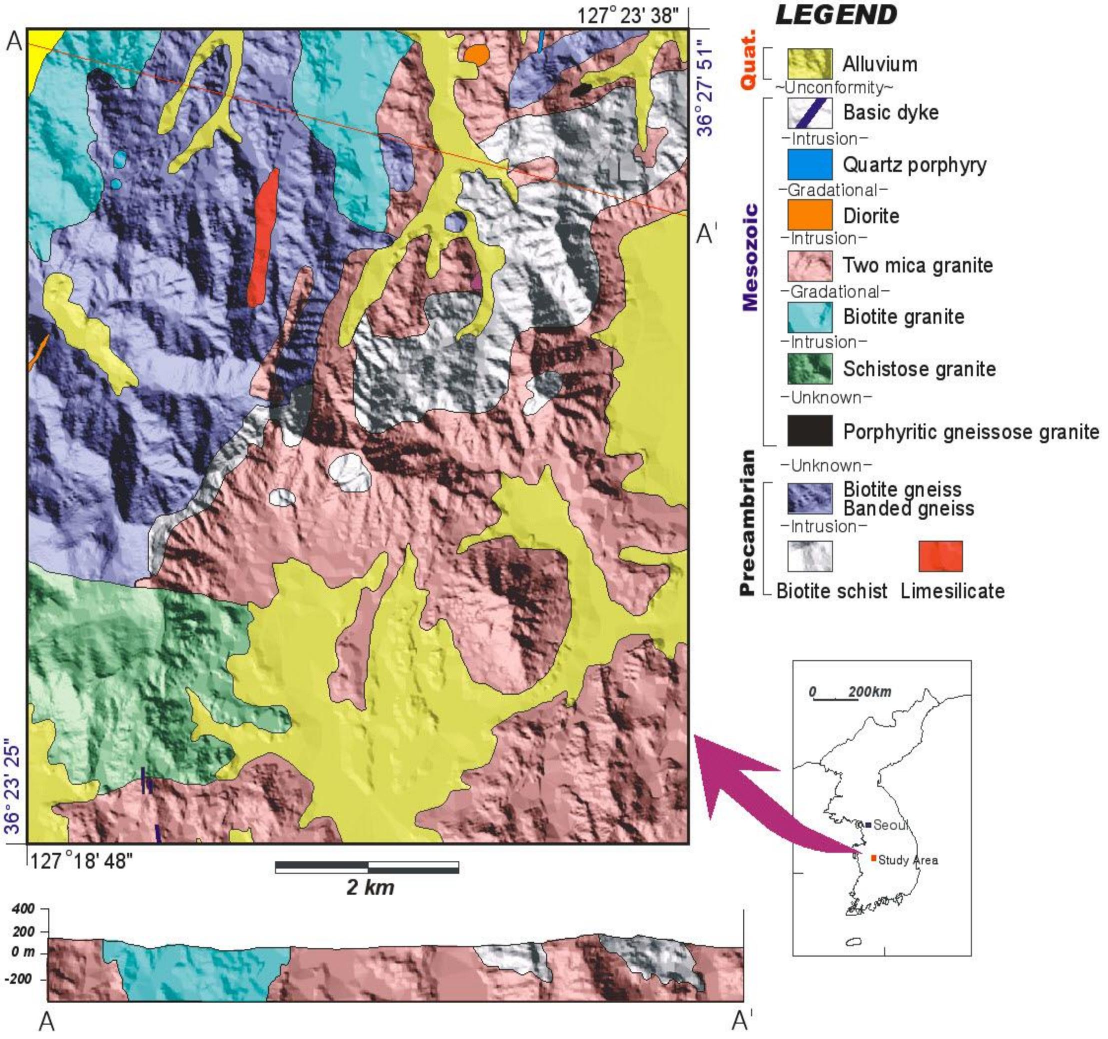


Figure 3-3. Location and geologic map of KURT site.

The mineralogy of fracture filling mineral were investigated from the borehole core samples. Most of the fractures are characterized by the existence of mineral coatings on the fracture surfaces. The fracture filling minerals are intergrown with each other. Illite, laumontite, calcite, chlorite, epidote, and montmorillonite were identified as fracture filling minerals. Laumontite (zeolite mineral) is very widely produced among the fracture-filling minerals. While a large amount of illite was not generated, it has the highest frequency of occurrence. The frequency of calcite is lower than that of the other fracture-filling minerals. Chlorite was mainly produced as an altered mineral on the fracture surfaces. The production of laumontite, epidote, and pyrite, in particular, suggests that the KURT site was influenced by hydrothermal alteration. According to observations using a scanning electron microscope (SEM), laumontite of a typical columnar crystal type and the illite and kaolinite of plate-type crystals were identified. In addition, chlorite and montmorillonite were produced as in a typical plate-type crystalline aggregation and typical honeycomb-type structure, respectively. Other fracture filling minerals identified in the cores include kaolinite, clinozoisite, pyrite, and iron oxides.

3.1.3 Boreholes in the KURT site

There are many boreholes at the KURT site (Figure 3-4). The lithological, mineralogical, rock mechanical, hydrogeological, and hydrogeochemical characteristics were investigated in these boreholes. Especially, a long-term monitoring of the groundwater pressure and chemical variations using a multi-packer (MP) system in DB-1 (SolExperts system, Switzerland) and YS-1 (Westbay system, Canada) boreholes was carried out. However, hydrochemical monitoring of YS-1 borehole has been stopped since 2006 due to the problem of MP system and grouting effect. The hydrochemical differences of YS-1 borehole were mainly resulted from the grouting activity, which carried out before MP installation on the fracture zone around GL-115m with Portland cement, where the borehole was collapsed after the drilling and hydraulic testing.

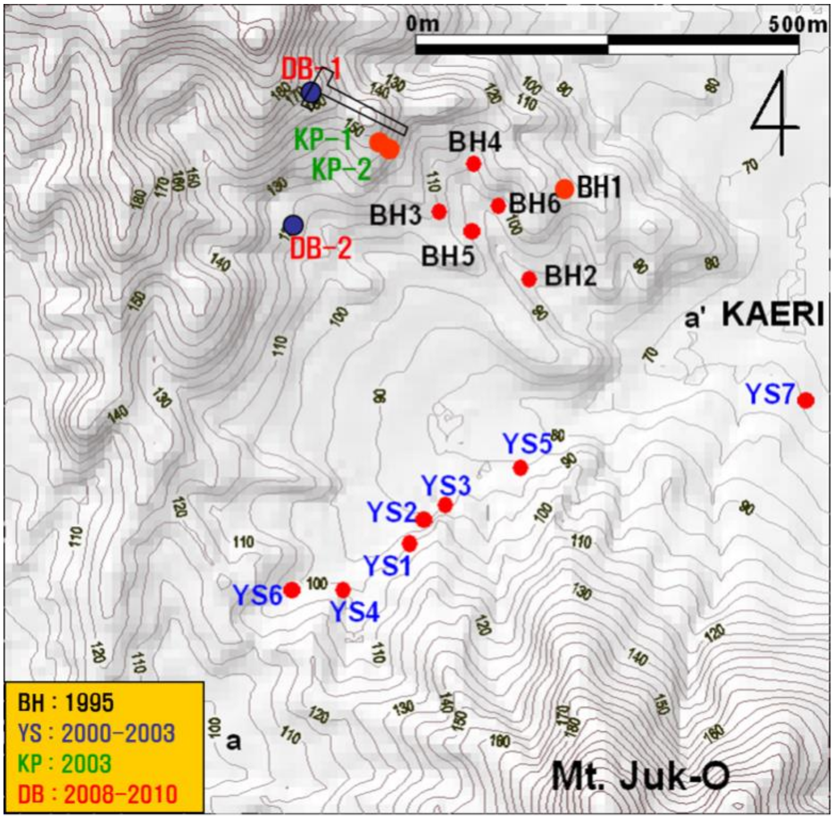


Figure 3-4. Location of boreholes around KURT

KAERI has been carrying out geoscientific researches at the KURT site since 1997. The main site investigation activities consist of the baseline geological, hydrogeological, geochemical, and rock mechanical properties of the host rock. For the geoscientific studies, the main goals are as follows:

1. Improve the geoscientific investigation technologies for the site characterization
2. Provide geoscientific data for system development and SA studies
3. Develop a detailed site descriptive model at the field-block scale

To achieve the goals, prior to the KURT project (~2002), a surface-based site investigation, i.e., lineament analysis, geophysical survey, shallow borehole investigation, hydraulic test, and geochemical exploration were performed. During this stage, BH and YS series boreholes were drilled for a field-scale investigation. The depth of these boreholes ranged from 100 to 500 m. Among them, all BH and some YS boreholes have been abandoned by the problem of long-term borehole management, i.e., collapse.

A detailed geological survey was performed in 2003 and 2004 during the design phase of the KURT facility. Data was obtained from the YS boreholes from 2003 to 2006 and KURT construction were analyzed and evaluated based on the results of the surface-based and YS-borehole investigations. In addition, KP-1 and KP-2 boreholes were investigated for the design of the KURT facility in particular prior to construction.

To evaluate the permeability of the fractured rock mass, a constant injection and a drawdown test at each monitoring interval were conducted using a double packer system at the BH, YS, and KP series boreholes (Kim et. al., 2002; Park and Bae, 2005).

The purpose of the underground characterization during the construction phase was to collect and integrate the geoscientific data to establish a hydro-structural framework of KURT as well as a baseline database for the hydrological isolation and retardation functions at the block scale. The main activities during the construction phase consisted of tunnel mapping (window and scan-line mapping), monitoring of the inflow rates and groundwater level variations, and the geochemical characterization of groundwater, rock, and fracture fillings. These results provided the baseline of geological input data for the design and preparation of in-situ experiments conducted in the tunnel.

During the operation of the KURT, DB-1 borehole was drilled at a depth of 500 m inside the tunnel to investigate deep geological environment of the Korean reference disposal concept. Based on the results from the investigation of DB-1, DB-2 borehole was drilled to a depth of 1,000 m outside of the tunnel to evaluate a main water conducting feature, which was identified during the DB-1 borehole investigation.

Additional geophysical surveys inside and outside of the tunnel, hydrogeological investigations (hydraulic testing and groundwater sampling), geophysical loggings, and VSP explorations in DB-1 and DB-2 boreholes were performed for developing geological model of the KURT site. These results were used to evaluate a conceptual hydrogeological model and a groundwater flow simulation (KAERI, 2000, 2009a, 2009b, 2009c).

The main objectives of the geoscientific studies conducted during the operation stage are to develop hydrogeological investigation techniques for a deep groundwater system, and to establish a geological and hydro-structural model at the field scale, as well as a fracture network model at the block scale. Both surface-based geological data and tunnel mapping data are integrated for a geosynthesis analysis, which is used to generate an updated geological and hydro-structural model. Several pieces of equipment and techniques, such as undisturbed groundwater sampling, hydro-testing of the artesian well condition, and sequential hydro-testing methods, were developed for a deep borehole investigation.

YS boreholes

YS series boreholes were drilled for a field-scale investigation prior to the KURT project. The following investigation methods were used to obtain a variety of geological information from the YS boreholes.

1. Core logging: Information for lithological varieties, visual inspection of fracturing and fracture conditions. More detailed analysis for the filling materials and minerals coating the fracture are carried out..
2. Televiewer logging (BHTV): the characteristic features observed from the BHTV images are primarily the fracture orientation, types of fracture (open, filled), average frequencies of fracture and aperture distribution.
3. Hydraulic testing during drilling: Constant pressure injection tests with a 10m interval for the selected zones were carried out during the interruptions of the drilling.
4. Groundwater monitoring in boreholes: The multipacker system (Westbay Co, Canada) was installed in the selected boreholes. The following items are periodically monitored.
    - Groundwater pressure monitoring from the packed-off sections
    - Groundwater sampling from each packed-off section
    - Water level changes of the open boreholes are obtained by an automatic recording system.
5. Hydrochemical investigation:
    - Sampling and analysis during the drilling: In conjunction with the hydraulic tests during the drilling
    - Long term monitoring of groundwater chemistry: Groundwater samples collected from each isolated section in the MP system are analyzed the following;
        - Index properties (pH, Eh, EC, T, DO, TDS)
        - Major/minor elements
        - Isotopes (18O, 2H, 3H)

DB-1 and DB-2 boreholes

During and after the KURT construction, Total 11 boreholes from 20 to 500 m depth were drilled within the KURT for hydraulic test, hydraulic and hydrochemical monitoring and sampling. Among them, the DB-1 borehole was drilled in vertical direction up to 200 m below tunnel bottom of KURT in 2006 and extended up to 500 m in vertical direction during 2007. The main objectives of deep drilling of DB-1 borehole are

1. To develop the hydrogeological and hydrochemical investigation techniques of deep borehole,
2. To obtain the detailed hydrogeological and hydrochemical parameters to understand the deep geological environment of KURT site,
3. To revise the hydro-structural model of KURT site.

DB-2 borehole was drilled to a depth of 1,000 m at southeastern part located outside of the KURT (Figure 3-5) to evaluate a main water conducting feature, which was identified during the DB-1 borehole investigation. The main objectives of DB-2 borehole are

1. To better understand deep geological, hydrogeological and geochemical characteristics around KURT site,
2. To estimate the hydrogeological characteristics of fracture zone with confidence building,
3. To revise the geological and hydrogeological model
   - Confirmation of fracture zone extension and revision of location of fracture zone,
   - Estimation of hydrogeological properties of fracture zone in DB-02 site.

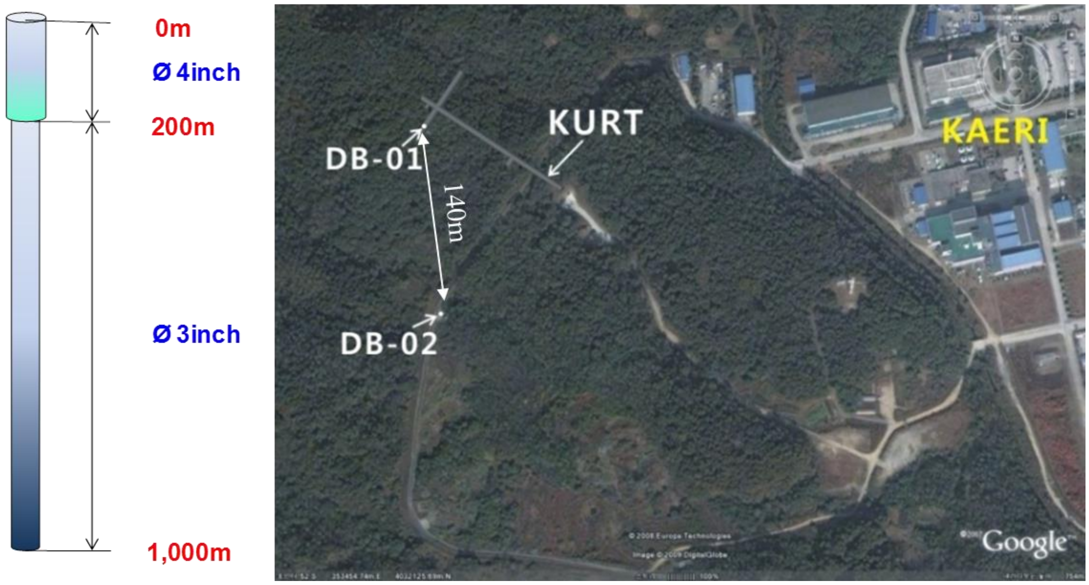


Figure 3-5. Specification of DB-2 borehole and its location in KURT site

Data on the actual descriptive models of the site were collected from the deep borehole investigations of DB-1 and DB-2. The most important geological information for evaluation was the influence of fracture zones on the groundwater flow and the vertical distribution characteristics of the hydrogeological and geochemical properties along the depth. To investigate the vertical variations of the physical properties of the rock mass and permeable features in the DB-1 borehole, temperature, electrical conductivity, SPS (suspension PS logging), full wave sonic, electric resistivity, and gamma logging analyses were carried out.

3.1.4 Current In-situ Test and Experiments in KURT

During phase I (2006~2011), the following in situ tests and experiments were carried out after the successful completion of construction in Nov. 2006. Figure 3-6 shows the location of in situ tests and experiments and the associated boreholes.

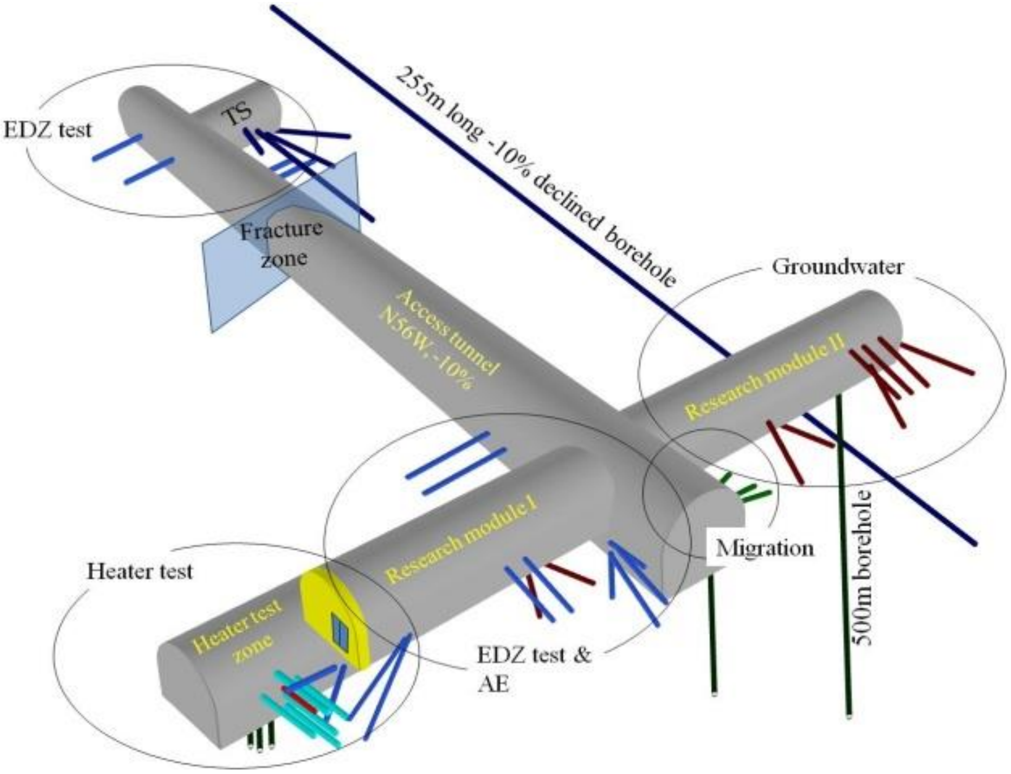


Figure 3-6. Location of in situ tests and experiments with related boreholes at KURT

Single-hole-heater test

HLW will generate heat when the radioactive materials in the waste are decaying. Because of this decay heat, the surrounding rock temperature will increase and this will result in a thermal stress, deformation, and mechanical strength change around a tunnel. It will also influence the groundwater flow pattern and geochemical condition. Such a change over a long period of time will affect the long term performance of the engineered barriers and deteriorate repository's safety.

For the single-hole-heater test, a 5 kW heater was installed in a heater hole, which has a diameter of 11cm, and about 100 temperature sensors were installed inside the rock surrounding the heater. The heater temperature was controlled to be increased step by step to 90°C. The power input, heater, air and rock temperatures, rock displacement, and rock stress were measured to investigate thermo-mechanical responses of the rock mass during the heating phase.

EDZ characterization

An excavation disturbed zone, in which the physical and chemical properties are changed from the original properties, is developed around a tunnel during or after an excavation. This zone influences the mechanical stability and groundwater flow around a tunnel. In the planned EDZ test, the rock mass property and in-situ stress changes were measured to determine the characteristics of the EDZ. The rock cores collected before and after the tunnel excavation were investigated to evaluate thermal and mechanical property changes. Different geophysical tests were also applied to determine the size of EDZ.

From the study, the primary parameters affecting the development of the EDZ were derived and their thermal, hydraulic, and mechanical properties were determined. These were used for a computer modeling for evaluating the stability and disposal safety of a proposed underground repository.

Solute and colloid migration experiments through a rock fracture

The migration and retardation processes of solutes and colloids through rock fractures are important for the safety assessment of a HLW repository. In-situ migration experiments are necessary to understand and demonstrate the migration processes of radionuclides and colloids in deep disposal environments. The migration experiments have been performed by dipole flow experiments between two connected boreholes connected using non-radioactive non-sorbing solutes such as eosine, uranine, and bromide and sorbing solutes such as Rb(I), Ni(II), Sm(III), and Zr(IV).

For the migration experiments, several boreholes were drilled, fractures were characterized, and in-situ experimental system was installed in the KURT. Colloid migration experiments using synthetic latex colloids with different sizes were performed in the same experimental area in order to characterize the colloid migration and filtration processes and to validate colloid migration models through a fractured rock. These in-situ migration experiments were also supported by the international joint study of CFM (Colloid Formation and Migration) project in Grimsel Test Site, Switzerland.

Physico-chemical properties of natural groundwater colloids sampled from a borehole with a multi-packer system in KURT characterized by using various analytical methods such as ICP-MS, TEM/SEM, PCS (Photon Correlation Spectroscopy), and mobile-LIBD (Laser-Induced Breakdown Detection).

Development of site investigation techniques

Hydraulic and hydrochemical investigations using deep boreholes require a QA(Quality Assurance) procedure. Through the planned site investigation tests, the QA procedures for various borehole tests as well as deep geological survey techniques are being developed. From this research, it is expected to be able to secure various techniques related to a deep borehole drilling, geological survey, rock and groundwater sampling, hydrological testing, borehole logging and analysis, long-term hydrological and geochemical monitoring, and so on.

Long-term corrosion experiment

Long-term corrosion rate of disposal canister materials and the effect of DO, Eh, and pH on the corrosion behavior were evaluated in the KURT. Groundwater from a deep borehole in KURT was transferred to a titanium vessel continuously to simulate a deep geological repository condition.

Hydrogeological evaluation and long-term monitoring

To build the hydrogeological model around KURT, the geological model was constructed before carrying out the hydrogeological investigation. KAERI has been performing several geological investigations such as geophysical surveys and borehole drillings since 1997. The DB-1 borehole, which has 500 m depth inside the left research module of the KURT, was drilled to confirm and validate the results from a geological model.

To evaluate the hydrogeological characteristics, the hydrogeological properties around KURT based on the geological model should be understood. The hydrogeological evaluations around the KURT include hydraulic properties for the different rock domains (fracture zones and rock mass), the groundwater conditions on the site and the processes that govern the natural flow of the groundwater. These evaluated results finally were used to construct the hydrogeological model. Therefore, the hydrogeological model mainly provided the information of the permeability of fracture zones and fractures, the flow porosity and storage coefficient, the distribution of hydrogeological data of the surface ecosystems.

Monitoring is an important aspect of the development and operation of a nuclear waste repository starting from the initial site characterization and continuing through to closure and sealing of the repository and possibly longer. Monitoring provides important data that feed into safety assessment calculations, either as input data or as information that can be used to confirm and refine predictions.

A network of boreholes and several deep boreholes equipped with long-term monitoring systems have been established in the KURT and groundwater samples have been analyzed in specified time intervals. In the KURT, continuous groundwater monitoring has been performed using multiple packer systems with multiple test intervals and interval accesses of the system as well as estimated water outflow. Monitoring equipment has been successfully tested in a large number of in-situ experiments in the KURT. Long-term monitoring of hydrogeological and geochemical parameters and the site descriptive hydro-structural modeling have been carried out.

International collaboration project with UFDC-SNL

KAERI investigated the influence of groundwater pressure change on a fracture aperture size during a hydraulic test. Fracture aperture controls the fracture transmissivity. Groundwater flow through fractures is a major pathway for radioactive contaminants to migrate from a subsurface repository to the biosphere. The cubic law relates transmissivity of a fracture to the cube of its aperture; a relatively small aperture change can lead to a large change in the flow rate and fracture transmissivity. While conducting hydrogeologic characterization, small changes in water pressure are applied, and they may affect fracture aperture and well testing results. To evaluate the influence of changes in water pressure on fracture aperture, an experimental borehole was drilled at the KURT, and a series of field experiments, where the aperture change due to water pressure change is directly observed under various water pressures, was conducted.

Another research is a correlation between the streaming potential (SP) signal and fracture flow. Streaming of water through pores and fractures in the ground produces an electric potential gradient, called a streaming potential (SP), along the flow path. Unlike for other geophysical methods, there is a direct link between SP and groundwater flow. The primary objective of the work is to determine hydraulic properties and behavior of a 3D subsurface volume of saturated fractured rock using hydraulic head and streaming potential data. To accomplish this objective, at the tunnel or drift scale we need to conduct pumping test with simultaneous monitoring of hydraulic head and streaming potentials. The KURT facility allowed a unique opportunity to create a medium-scale coupled hydrogeophysical experiment in fractured granite.

3.1.5 Phase II In-situ Test and Experiments Plan in KURT

Five-year R&D program for HLW long-term management system development during 2012 to 2016 (Phase II) focuses on

1. Enhancement of the performance of EBS,
2. Development of safety cases based on the KURT environment,
3. Establishment of the infrastructure for in-situ demonstrations at KURT,
4. Characterization of the MWCF: Hydrogeology, Geochemistry, Transport property

During phase II (2012–2016), additional intensive experiments on hydrogeological characterization of MWCF and in situ long-term performance tests on a 1/3 scale engineered barrier system are major experimental research items to be executed at the KURT facility. The current dimensions of the research modules are limited, and thus the KURT facility needs to be extended for the execution of the planned tests and experiments during phase II. The KURT extension plan for Phase II research was accepted by the Government in 2012.

Three pilot boreholes were drilled along the extension direction for the design of the tunnel. Two monitoring boreholes (MB-1 and MB-2) were drilled outside and inside the KURT based on the results of hydrogeological investigation and modeling (Figure 3-7). For long-term monitoring of the groundwater pressure and chemical variations, multi-packer systems (SolExperts system, Switzerland) were installed in monitoring boreholes. Monitoring sections were identified by the results of borehole investigations.

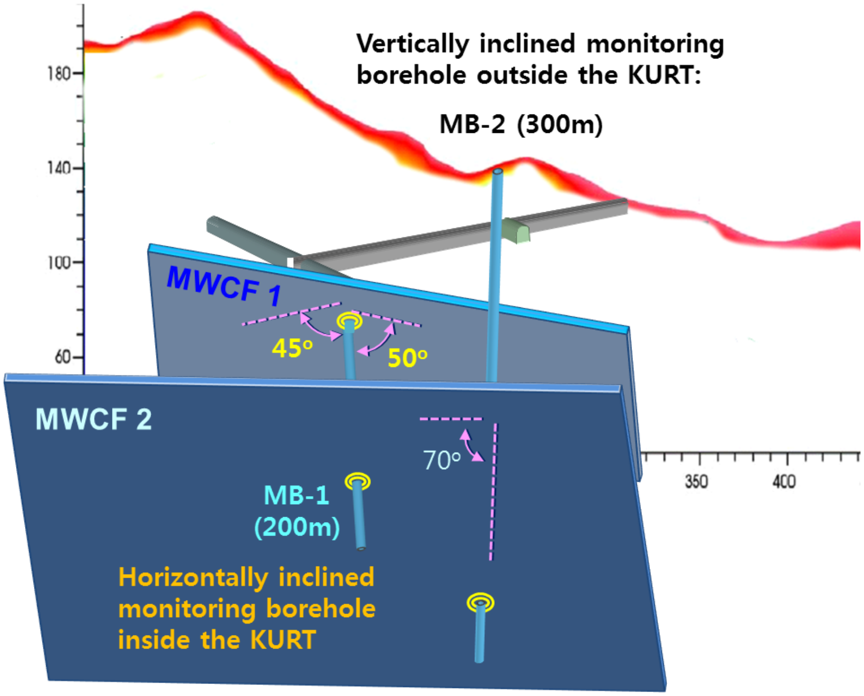


Figure 3-7. Layout of two monitoring boreholes for tunnel extension of KURT

The design of the tunnel layout and construction method was optimized by March 2013. The design requirements for KURT were as follows:

1. Site investigation should be focused on the possible extension area,
2. Extension tunnel layout should be optimized depending on the geological condition, especially distribution characteristics of MWCF,
3. Predictive geological and rock mechanical model should be presented to ensure the extension concept.
4. At least, 6 research modules should be constructed within limited extension area on condition of minimizing the interference effect between adjacent research modules.

Figure 3-8 shows an example of the potential tunnel layouts, which could be modified depending on the results from site investigations. Total length of extended horizontal tunnel will be approximately 288 m with 165 m looped shape access tunnel, 42 m connection tunnel and 4 research modules with a total length of 81 m. Tunnel shape and dimension is designed as horseshoe shape with 6m (W) x 6m (H) (same as Phase I tunnel). Maximum depth of research module will be 130 m from the peak of the mountain.

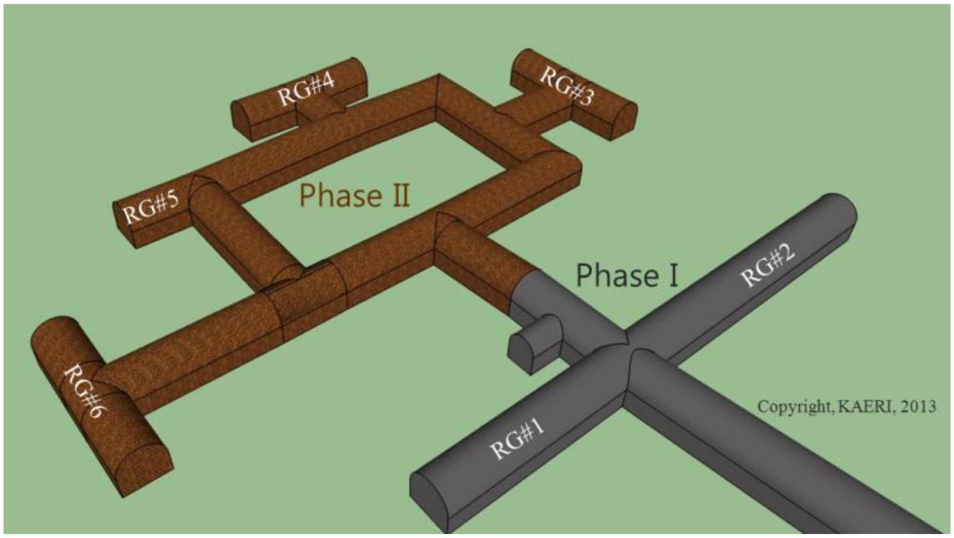
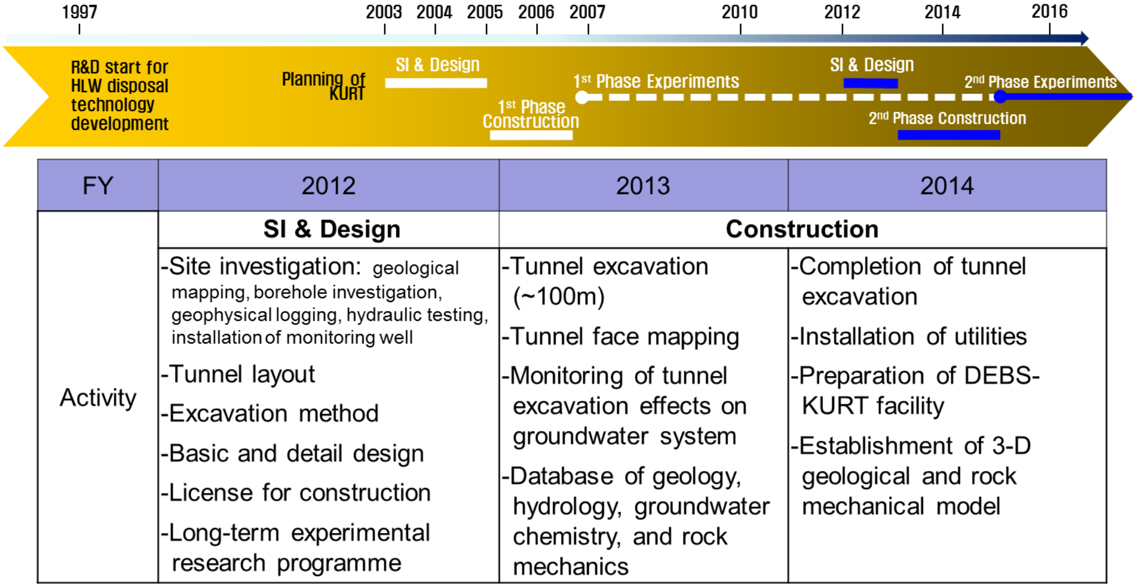


Figure 3-8. An preliminary layout for tunnel extension of KURT

The tunnel and additional utilities will be started on mid-2013 and completed by 2014. The overall extension schedule and related activities are shown in Figure 9.



FY	2012	2013	2014
	SI & Design	**Construction**	
Activity	-Site investigation: geological mapping, borehole investigation, geophysical logging, hydraulic testing, installation of monitoring well -Tunnel layout -Excavation method -Basic and detail design -License for construction -Long-term experimental research programme	-Tunnel excavation (~100m) -Tunnel face mapping -Monitoring of tunnel excavation effects on groundwater system -Database of geology, hydrology, groundwater chemistry, and rock mechanics	-Completion of tunnel excavation -Installation of utilities -Preparation of DEBS-KURT facility -Establishment of 3-D geological and rock mechanical model

Figure 3-9. Extension schedule and related activities for Phase II

Planned Tests and Experiments in Phase II

Phase II tests and experiments proposed by the KURT research fellows include:

1. Hydrological and hydrochemical monitoring: basic activities during construction and operation stage,
2. Long-term corrosion experiment: bentonite and copper canister using deep groundwater,
3. Establishment of site descriptive model: The model should be revised base on the data obtained during the excavation.
4. MWCF characterization: before, during and after the excavation
5. In-DEBS: design and preparation for 1/3 scale EBS performance tests will be initiated in 2013, and in-situ tests will be started in late 2014.
6. International collaboration project with UFDC (SNL): SP test, started in FY2013.

Figure 10 shows all in-situ tests and experiments in KURT and overall schedule for Phase II.

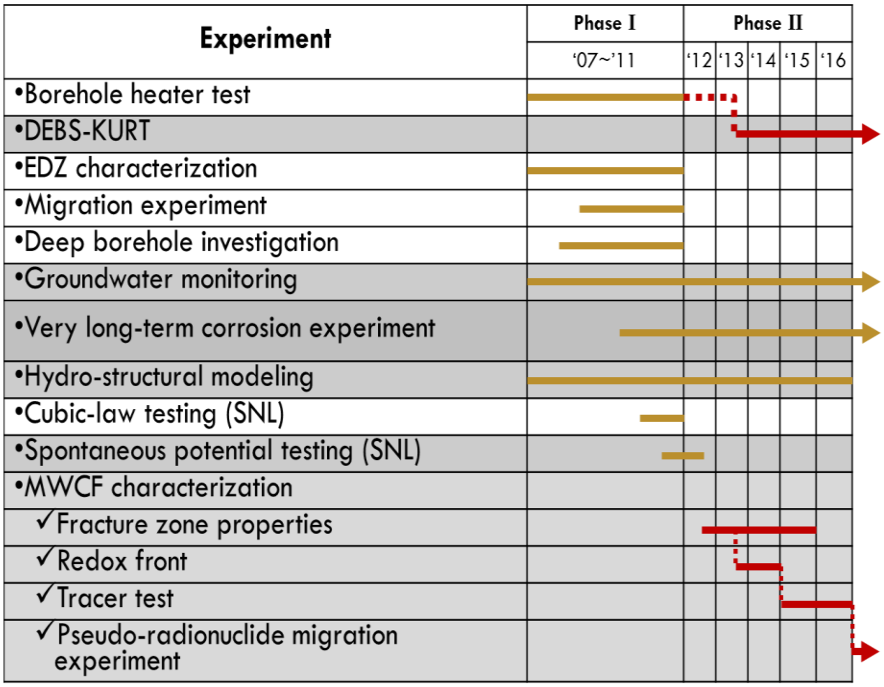


Figure 3-10. Planned tests and experiments in Phase II

3.1.6 Key Techniques to Develop Using Deep Borehole (DB-2) at KAERI Site

KAERI identified key techniques which should develop using deep borehole (DB-2) at KAERI site and grouped them into four categories, i.e., in-situ measurement and data acquisition, rock mechanical investigation, microbiological and biogeochemical evaluation, and solute migration.

KAERI will provide UFDC-SNL with new fracture, hydrologic and hydrochemical data from the KURT site. When evaluating the current hydrological/geochemical data of KURT site is completed, SNL and KAERI will discuss target investigation items and their priority based on the key techniques proposed in this chapter, then the finalized key techniques will be proposed.

Development of in-situ measurement and data acquisition techniques

Objectives:

- Better understanding of deep hydrogeological and geochemical characteristics and uncertainty reduction in evaluating deep geological environments of granitic area

Key techniques:

1. *Development of in-situ measurement equipment for hydrological and hydrochemical parameters at high pressure conditions in a deep borehole*: The size of equipment should be smaller than the diameter of DB-2 borehole (~ 3 in) and focused on non-destructive techniques. KAER and SNL are evaluating the current hydrological/geochemical data. We will discuss target investigation item(s) and develop new techniques as needed.
2. *Development of groundwater sampling and monitoring technique from very low water conductivity zone of a deep borehole*: Hydrochemistry of deep groundwater is important for the evaluation of water-rock interactions, oxidation/reduction state, oxidation-reduction buffering ability and complex interactions of hydro-mechanical and hydrochemical phenomena in deep condition. Nevertheless, groundwater sampling and monitoring for very low water conductivity zone in a deep borehole is still challenging.
3. *Development of techniques for remote measurement of hydrochemical and hydrological properties from a deep borehole*: Because monitoring system using electric wires for data measurement and transfer usually has its mechanical uncertainty as well as limited durability. Long-term monitoring system using a remote system or multi-functional materials such as optical fiber could reduce uncertainty for measurement and transfer of real time in-situ data from a deep borehole during a very long monitoring period. A feasibility study and research for related sensors and output signal processing algorithm should be preceded.
4. *Alternative techniques for earthquake and micro-movement observation in a deep borehole*

Development of rock mechanical investigation techniques

Objectives:

- Evaluation of mechanical characteristics and construction of rock mechanical models in deep geological environments of granitic area

Key techniques:

1. *Development of an in-situ rock stress measurement strategy*
2. *Techniques for mechanical tests in deep boreholes to determine in situ stress state*
3. *Evaluation techniques for geomechanical development and long-term behavior of the excavation disturbed zone and the surrounding rock mass in a deep borehole*
4. *Evaluation techniques for geochemical development and long-term behavior of the excavation disturbed zone and the surrounding rock mass in deep borehole*

Development of evaluation techniques for microbiological and biogeochemical effect in deep environment

Objectives:

- Evaluation of microbiological and biogeochemical effects in deep environments of granitic area and development of the integrated biochemical and geochemical modeling tools

Key techniques:

1. *Evaluation techniques for microbiological and biogeochemical effects on the variation of hydrological properties of the fracture network in deep environments*: Biomass accumulation or biomineralization are usual phenomena which can be caused by microbiological and geochemical reactions in the groundwater system. They could affect all elements related to the stability and safety of a deep geological disposal system, especially the groundwater flow system. The development of techniques for understanding, prediction, prevention and reduction is strongly required for the long-term operation of deep underground facilities.
2. *Evaluation techniques for microbiological effects on oxidation-reduction conditions in deep environments*

Development of evaluation techniques for solute migration and natural analogue study

Objectives:

- Evaluation of solute migration properties in deep geological environments of granitic areas

Key techniques:

1. *Techniques for the characterization of the transport property of a water-conductive fractured zone and the hydraulic connectivity among fractures in a crystalline rock*: Laboratory scale test should be preceded for evaluation of the effect of a stagnant zone on solute transport in a fracture. Experimental devices to minimize the experimental errors should be developed prior to in-situ tracer test. This technique could be commercially applied to understanding the fracture networking and its connectivity through a tracer test before and after deposition hole construction of a deep geological repository.
2. *Techniques for natural analogue studies using deep boreholes*: Natural analogues such as uranium deposits preserve information about physical and chemical processes that may be relevant to nuclear waste isolation in a geologic repository. This information could be useful for the repository performance assessment model validation and confidence building (Wang, 2013). In the case of existence of anomaly zone for radionuclides in a deep borehole, the natural analogue study could be carried out and related techniques such as monitoring and sampling techniques should be developed in relation to the development of in-situ measurement and data acquisition techniques.

Other techniques

1. *Evaluation technique for the long-term evolution of EBS materials and their impacts on the groundwater chemistry*: This technique will help to better predict the long-term

evolution of the repository materials (bentonite, cementitious materials, canister materials etc.) in granitic groundwater chemistry.

3.2 Preliminary Research on Correlation between the Self- potential (SP) and Solute Transport

3.2.1 Introduction

Characterizing the spatial distribution of hydraulic properties of porous media and fractured rock is an essential step toward high-resolution predictions of water flow and contaminant transport near a radioactive waste repository in a geological medium. Generally, the hydraulic characterization of a geological medium has been investigated by traditional aquifer test methods such as pumping, slug and tracer tests. Unfortunately, only a few wells are available for a given flied test or monitoring program, which causes the relatively insufficient information to understand the groundwater flow and solute transport in an aquifer and to estimate the hydraulic parameters. Moreover, these methods are intrusive and consequently the hydrological system is perturbed by drillings.

Geophysical approaches instead aim to use non-intrusive techniques to obtain a large amount of information on subsurface and with low cost. In the last few decades hydrologists have increasingly begun to use geophysical information to estimate groundwater flow parameters (Cassiani and Medina, 1997; Troisi et al., 2000; Kemna et al., 2002; Slater and Lesmes, 2002; Binley et al., 2005; Linde et al., 2006; Koestel et al., 2009). However, the self-potential (SP) method is the only geophysical technique that is sensitive to the movement of groundwater in real time. Indeed, the streaming of water through pores and fractures in the ground can produce a natural electrical potential (called streaming potential) along the flow path. Therefore, unlike for other geophysical methods, there is a direct relation between SP signal and groundwater flow. A number of recent studies have shown the high interest in the SP method for applications in hydrogeophysical problems associated groundwater. These applications include the identification of the direction and rate of groundwater flow in the vadose zone and in shallow unconfined aquifers (Doussan et al., 2002; Revil et al., 2003), the interpretation of pumping and infiltration tests (Rizzo et al., 2004; Suski et al., 2004; Titov et al., 2005; Straface et al., 2007; Malama et al., 2009), and the determination of the capillary fringe using harmonic pumping tests (Maineult et al., 2008; Revil et al., 2008).

Although the SP method has seen use in quantifying properties associated with porous media (e.g., aquifer transmissivity and storativity), it has only been used in preliminary studies to delineate discrete fractures and anisotropic flow patterns (Hunt and Worthington, 2000; Wishart et al., 2006; Suski et al., 2008). Recently, Lee et al. (2013) developed a semi-analytical solution of the self-potential field related to transient hydraulic response of a fractured rock aquifer to constant rate pumping through a fully penetrating well. This analytical solution has been applied to field data of self-potential associated with the pumping phase of an aquifer test recorded at the Korea Underground Research Tunnel (KURT), which yield the hydraulic conductivity and specific storage values that compare well to analysis results by aquifer test software. In this study, the pumping tests were very precisely controlled by using the specially-manufactured device for maintaining the pumping rates, because the pumping rates of fractured rock aquifer in KURT was very small and irregular compared to those of general porous medium. Contrary to the correlation between the self-potential and hydraulic property of an aquifer, the correlation between the self-potential and transport property has not been investigated thoroughly to our best knowledge.

The objective of this study is to obtain a mechanistic understanding of the coupling of electrochemical processes with hydrologic flows in a fractured rock. A preliminary tracer test in a laboratory scale is performed with SP signal monitoring. This testing will support a SP test at KURT, which will be started after KURT expansion and is expected to support the Used Fuel Disposition (UFD) effort on developing advanced methods for characterizing an excavation-disturbed zone (EDZ).

Figure 3-11: Sand box for the preliminary tracer test

3.2.2 Preliminary tests

Figure 3-11 shows the sand box for this study. A 1 m long x 0.5 m wide x 0.4 m high hypothetical aquifer is prepared by filling standard sand in the sand box, and reservoirs on either ends of the aquifer allow the variation of the ambient hydraulic gradient and thus the groundwater flow. With this sand box, a preliminary test was conducted to check if the self-potential at the aquifer can be detected with the prepared self-potential monitoring device and the device is sufficiently sensitive for detecting the change of water pressure. The aquifer was saturated with water, and the self-potential monitoring device was installed. Then, we drained water from the aquifer measuring the self-potential. Figure 3-12 shows the result of the preliminary test. As the water table decreases, the self-potential also decreases, which means that the installed device is sufficiently sensitive to detect the change of self-potential at the test aquifer.

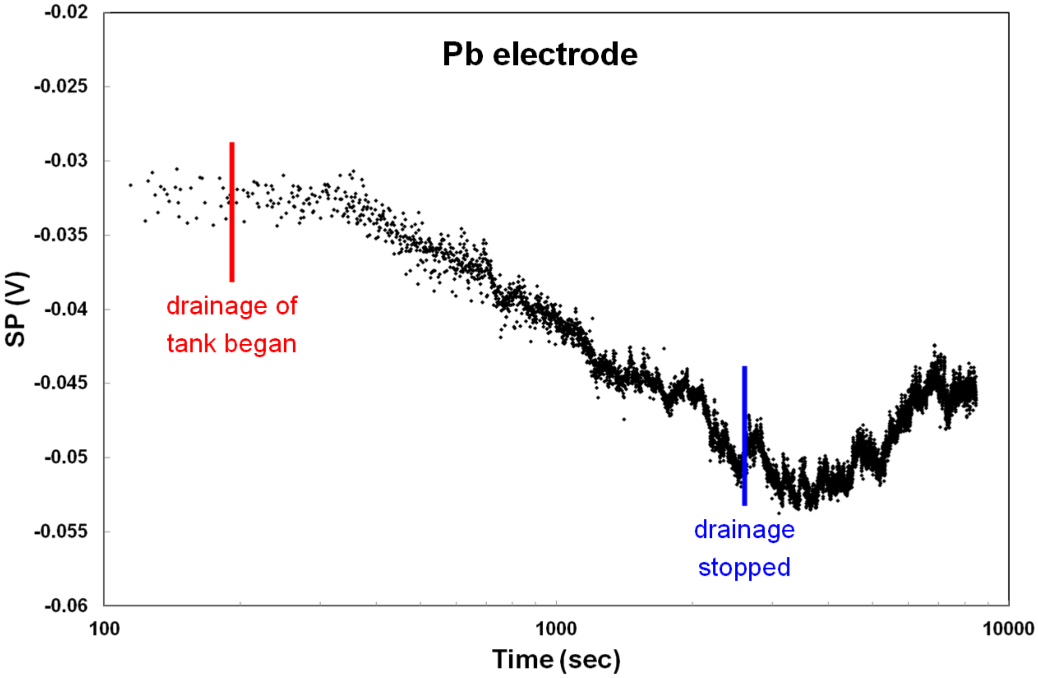


Figure 3-12: Change of SP in the sand box during drainage of water.

3.2.3 Future work

According to the research plan of this study, we will conduct the following experiments.

(1) Hydraulic test in the test aquifer: To characterize the hydraulic property such as the hydraulic conductivity, we will conduct a water flow test. A fixed hydraulic gradient will be imposed using the reservoirs on either ends of the aquifer, and the outflux will be measured at the downstream with a flow meter. From Darcy's law, we will constrain the hydraulic conductivity of the test aquifer.

(2) Tracer test in the test aquifer: Pb electrodes will be installed in a shape of a lattice with a distance of 10 cm to monitor the self-potential. Then, a groundwater flow in steady-state will be established. After the outflx and self-potential are stabilized, a solute will be injected at the upstream of the test aquifer and the concentration of the solute will be

measured at the downstream. The change of self-potential near the downstream and the breakthrough curve of the solute will be compared each other. Note that the concentration of the injected solute will be one of the system parameters of this study. Then, the correlation between the self-potential and the concentration or ionic strength of the injected solute will be inferred qualitatively.

(3) Test in the KURT. After the completion of the new excavation of the KURT, the test equipment will be transferred into the field to start a test on the actual EDZ of the tunnel. This testing will directly support the UFDC effort on developing advanced methods for characterizing an excavation-disturbed zone (EDZ). KAERI will be responsible for instrumentation, field testing and data acquisition. SNL and KAERI will work jointly on experimental design and data interpretation.

3.3 Technical Exchange at Fuel Cycle Alternative Working Group (FCAWG) Meeting

The Fuel Cycle Alternative Working Group under the Joint Fuel Cycle Studies bilateral between the Republic of Korea (ROK) and the United States (US) Department of Energy (DOE) held meeting from June 23 to June 25, 2014, at the Pacific Northwest National Laboratory in Richland, Washington.

Dr. Yifeng Wang from SNL discussed activities associated with the areas of mutual interest. During his discussion, he described advantages that the UFDC has identified with respect to crystalline host rock disposal systems. He also stated that since the ROK is still developing disposal concepts in crystalline (granite and gneiss), the US can test concepts at the ROK (including, but not necessarily limited to the KAERI Underground Research Tunnel). Since the ROK has not yet identified specific disposal concepts as has been done in European programs in crystalline host rock, experimentation by the UFDC can occur more openly without interfering with work in the ROK.

Dr. Wang also discussed the development of reference cases in the US and their applicability to the development of disposal systems in crystalline host rock. In these activities, site characterization data as being made available from the ROK has proven and should continue to prove valuable to the US program. SNL acknowledged the receipt of three technical reports from KAERI. The report on KURT site characterization data was incorporated into a UFDC level II milestone report last year. The other two reports will be incorporated into a UFDC milestone report this year.

Drs. Lee, Jung and Kim offered the following new deliverables to the US, all of which were welcomed by Dr. Wang who expressed the belief that they will continue to provide value to the US program:

1. The ROK will provide to the US the fracture properties on two ROK research sites (granite and gneiss) that will be benefical and useful to the US program [May 1, 2015]
    - Up to 500 m in depth where it is expected to be more fractured than in deeper crystalline environments, and

  - 500-1000 m in depth where it is anticipated that the fracturing will be less than in shallower environments.
2. Continued work at KAERI and KURT through the contract funded by the US DOE UFDC through Sandia National Laboratories. Dr. Wang expressed an interest in using the newly excavated tunnel in KURT for flow and transport testing in major water conductive fractures.

3. A report on properties of buffer material from KAERI based research in the ROK [January 15, 2015]

4. Topographic data developed by the ROK to be provided to the US [December 3, 2015]

5. Crystalline parameters gathered by the ROK (May 1, 2015) including
   - Hydrologic properties such as K, T, etc.
   - Geochemical data (cation and anion data)

Dr. Wang discussed the analyses of fractured systems in crystalline environments, as well as R&D being conducted on buffer materials. He indicated the importance of the buffer materials in a crystalline host rock environment (as opposed, for example, to a salt or clay environment where the host rock tends to creep and encapsulate the waste packages). Since crystalline host rock does not creep, the engineered materials used to contain radionuclide migration become a significantly important aspect of the crystalline environment. Dr. Wang identified the following deliverables from the US to the ROK, all of which were accepted as being useful by the ROK.

1. Anion uptake and transport in compacted clay materials is an important issue in the evaluation of a crystalline rock repository. ROK expressed an interest in SNL's work on iodide sorption and transport. A high-level radioactive waste management conference paper on this topic will be made available to the ROK [October 31, 2014].

2. Discrete Fracture Model (DFM) tool that is being developed in the UFDC will be made available to the ROK, as well as the continuum model [October 31, 2014]

3. The UFDC has conducted a number of experimental and modeling tasks on the thermal limits of bentonite (Ca and Na) clays used in engineered barrier systems with results that seem to indicate that the previously held belief of a limit of 100 ^{o}C can be raised or eliminated. By raising the thermal limit in a repository, a greater flexibility is afforded to the system. The report will be made available to the ROK [October 31, 2014]

4. Milestone report at the end of FY 2014 that discusses R&D in engineered barrier systems, natural systems considerations and reference case development for crystalline host rock repository environment [October 31, 2014].

5. Milestone report at the end of FY2014 on thermodynamic data development for clays and cementitious materials will be delivered to the ROK [October, 2014].

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4. Summary

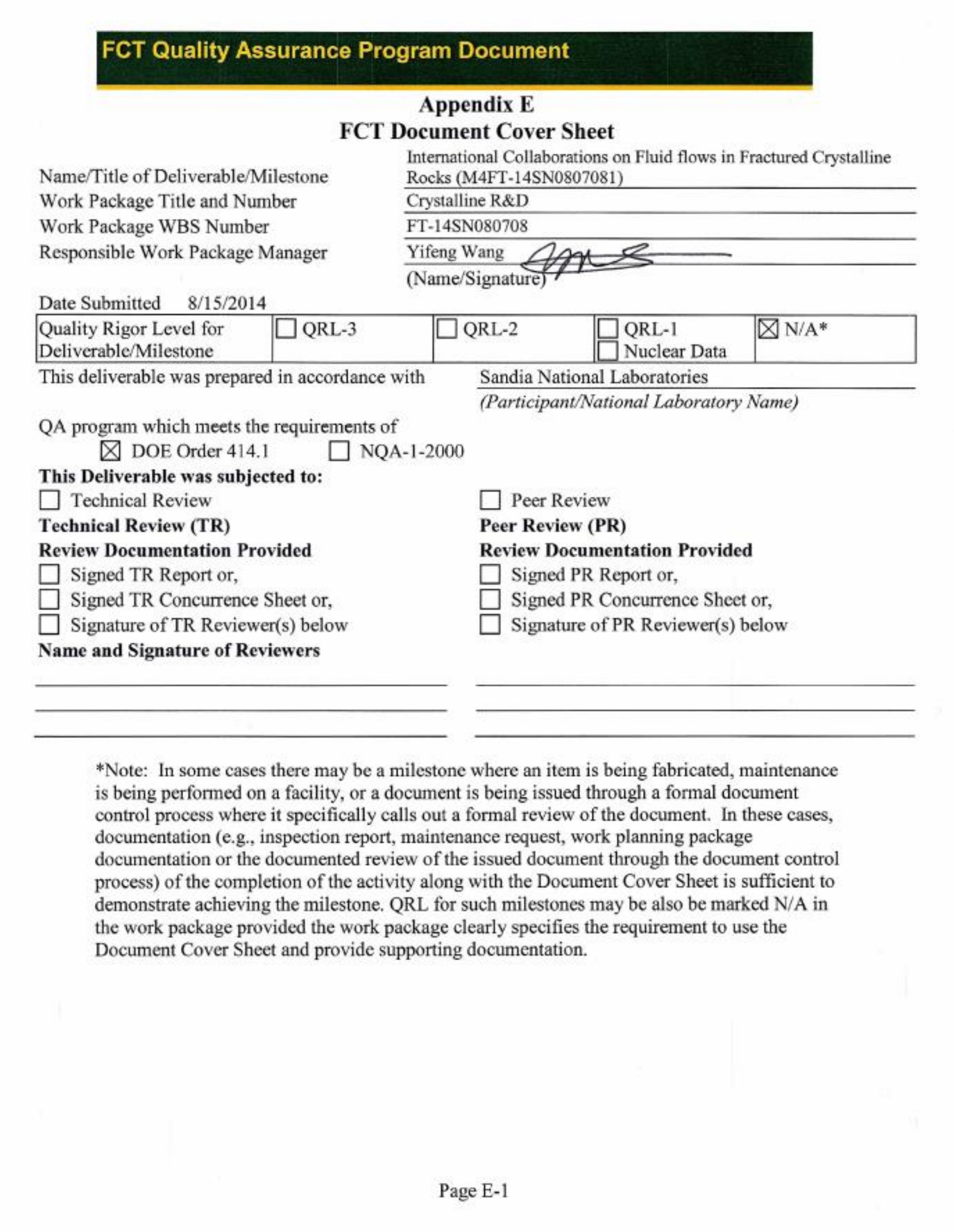
The international collaboration on the evaluation of crystalline disposal media at SNL in FY14 was focused on the following two activities: (1) simulations of flow and transport in Bedrichov Tunnel, Czech Republic as a part of the DECOVALEX program, and (2) KAERI Underground Research Tunnel testing in crystalline rocks. The major accomplishments include:

- DECOVALEX-Bedrichov Tunnel Tests: A lumped parameter model was developed for stable isotope, tritium and CFC-12 transport at the Bedrichov Tunnel site and modeled results were compared to measured data. The lumped parameter model consistently predicts heavier isotopic values observed at the site, indicating preferential recharge of winter precipitation. Code PFLOTRAN was used to simulate multiple environmental tracer concentrations in heterogeneous 2D and 3D domains. Fracture zone permeability was calculated by matching the steady tunnel discharge to the appropriate values given in the task description. The modeling results have demonstrated the potential of using both the lumped parameter model and the PFLOTRAN code for modeling flow and transport in fractured crystalline rocks. The comparison of modeling results among the participating DECOVALEX teams has improved the confidence for the intended use of the modeling tools.

- KAERI Underground Research Tunnel Test: Sandia National Laboratories (SNL) and Korean Atomic Energy Research Institute (KAERI) have developed a multi-year plan for joint field testing and modeling to support the study of high-level nuclear waste disposal in crystalline geologic media. The work for FY14 is focused on two tasks: (1) streaming potential (SP) testing, and (2) technique development for in-situ borehole characterization. For task 1, KAERI has completed the experimental setup and a first set of preliminary tests. This testing system will be transferred to the underground research laboratory once the new excavation in the KURT is completed. For Task 2, KAERI and SNL have developed a roadmap for the development of site characterization techniques for fractured crystalline rocks, especially the in-situ hydrological and geochemical measurements in boreholes.

- A technical exchange meeting was held under the Joint Fuel Cycle Studies (JFCS) bilateral between the Republic of Korea (ROK) and the US DOE. A list of deliverables for technical data exchange has been identified for next two years.

Future work will include: (1) helping to complete the final technical report for DECOVALEX-2015 Task C; (2) working closely with KAERI on the streaming potential testing in the KURT; (3) planning an actual field test at the KURT site for the development of in-situ measurement techniques in boreholes; and (4) formulating a plan for a joint flow and tracer test at the KURT using the newly excavated tunnel. In addition, we will ensure the delivery of the list of deliverables identified at the JFCS technical exchange meeting.



FCT Quality Assurance Program Document

Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone: International Collaborations on Fluid flows in Fractured Crystalline Rocks (M4FT-14SN0807081)
Work Package Title and Number: Crystalline R&D
Work Package WBS Number: FT-14SN080708
Responsible Work Package Manager: Yifeng Wang
(Name/Signature)

Date Submitted 8/15/2014

Quality Rigor Level for Deliverable/Milestone	☐ QRL-3	☐ QRL-2	☐ QRL-1 ☐ Nuclear Data	☒ N/A*

This deliverable was prepared in accordance with Sandia National Laboratories
(Participant/National Laboratory Name)

QA program which meets the requirements of
☒ DOE Order 414.1 ☐ NQA-1-2000

This Deliverable was subjected to:

☐ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
☐ Signed TR Concurrence Sheet or,	☐ Signed PR Concurrence Sheet or,
☐ Signature of TR Reviewer(s) below	☐ Signature of PR Reviewer(s) below

Name and Signature of Reviewers

*Note: In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity along with the Document Cover Sheet is sufficient to demonstrate achieving the milestone. QRL for such milestones may be also be marked N/A in the work package provided the work package clearly specifies the requirement to use the Document Cover Sheet and provide supporting documentation.